C55C-C54C-H54C	119.5(19)	C55C-C56C-C51C	120.9(3)
C54C-C55C-C56C	119.8(3)	C55C-C56C-H56C	122(2)
C54C-C55C-H55C	119.7(19)	C51C-C56C-H56C	117.3(19)
C56C-C55C-H55C	120.4(19)		

C2-C1-C6	120.0	C10-C9-H9D	109.5
C2-C1-C7#1	27.6(6)	C10-C9-H9E	109.5
C6-C1-C7#1	92.4(6)	H9D-C9-H9E	109.5
C2-C1-H1	120.0	C10-C9-H9F	109.5
C6-C1-H1	120.0	H9D-C9-H9F	109.5
C7#1-C1-H1	147.6	H9E-C9-H9F	109.5
C1-C2-C3	120.0	C11-C10-C9	113.2(6)
C1-C2-H2	120.0	C11-C10-H10A	108.9
C3-C2-H2	120.0	C9-C10-H10A	108.9
C2-C3-C4	120.0	C11-C10-H10B	108.9
C2-C3-H3	120.0	C9-C10-H10B	108.9
C4-C3-H3	120.0	H10A-C10-H10B	107.7
C5-C4-C3	120.0	C10-C11-C12	111.6(5)
C5-C4-H4	120.0	C10-C11-H11D	109.3
C3-C4-H4	120.0	C12-C11-H11D	109.3
C4-C5-C6	120.0	C10-C11-H11E	109.3
C4-C5-H5	120.0	C12-C11-H11E	109.3
C6-C5-H5	120.0	H11D-C11-H11E	108.0
C5-C6-C1	120.0	C13-C12-C11	109.6(4)
C5-C6-C7	115.8(5)	C13-C12-H12D	109.7
C1-C6-C7	124.2(5)	C11-C12-H12D	109.7
C6-C7-C1#1	31.8(7)	C13-C12-H12E	109.7
C6-C7-H7D	109.5	C11-C12-H12E	109.7
C1#1-C7-H7D	141.3	H12D-C12-H12E	108.2
C6-C7-H7E	109.5	C12-C13-H13D	109.5
C1#1-C7-H7E	92.0	C12-C13-H13E	109.5
H7D-C7-H7E	109.5	H13D-C13-H13E	109.5
C6-C7-H7F	109.5	C12-C13-H13F	109.5
C1#1-C7-H7F	92.0	H13D-C13-H13F	109.5
H7D-C7-H7F	109.5	H13E-C13-H13F	109.5
H7E-C7-H7F	109.5		

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+2,-z+1

Table 10. Anisotropic displacement parameters ($Å^2 x 10^4$) for 2 CCDC 164301 MSS14. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru1A	111(1)	86(1)	119(1)	-9(1)	-13(1)	0(1)
P1A	111(4)	101(4)	122(4)	-11(3)	-15(3)	-4(3)
O1A	140(11)	114(11)	144(11)	2(9)	-16(9)	7(9)
O2A	143(12)	132(11)	160(12)	32(9)	-48(9)	-7(9)
N1A	157(14)	101(13)	139(14)	-21(11)	-13(11)	1(11)
N2A	144(14)	125(14)	148(14)	-2(11)	6(11)	-14(11)
N3A	153(14)	117(13)	108(13)	-26(10)	-22(11)	-15(11)
N4A	168(14)	87(13)	116(13)	6(10)	-29(11)	-20(11)
N5A	114(13)	132(14)	119(13)	7(11)	-7(11)	-7(11)
N6A	159(14)	123(14)	127(14)	-22(11)	-1(11)	-8(11)
B1A	133(19)	169(19)	134(19)	-4(15)	21(15)	-27(15)
C1A	180(17)	93(15)	124(16)	-6(12)	-30(13)	44(13)
C2A	182(17)	126(16)	134(17)	20(13)	-39(14)	-13(13)
C3A	171(17)	133(17)	246(19)	37(14)	-99(15)	-24(13)
C4A	138(17)	124(17)	380(20)	-37(15)	-127(15)	39(13)
C5A	270(20)	240(20)	300(20)	-114(17)	-67(17)	44(16)
C6A	300(20)	380(20)	400(20)	-180(20)	-86(19)	57(18)
C7A	230(20)	330(20)	530(30)	-200(20)	-140(20)	93(17)
C8A	250(20)	137(19)	770(30)	-110(20)	-220(20)	9(16)
C9A	240(20)	175(19)	490(30)	-25(18)	-135(18)	3(15)
C10A	205(18)	116(16)	215(18)	22(13)	-43(14)	-83(13)
C11A	222(19)	180(18)	212(19)	-15(15)	-24(15)	-36(14)
C12A	230(20)	230(20)	320(20)	-69(16)	-36(17)	-17(15)
C13A	240(20)	240(20)	390(20)	-112(17)	54(18)	-92(16)
C14A	380(20)	216(19)	191(19)	-57(16)	48(17)	-142(17)
C15A	330(20)	183(18)	214(19)	-1(15)	-83(16)	-117(16)
C16A	161(17)	148(17)	122(16)	-39(13)	-25(13)	24(13)
C17A	139(17)	138(16)	123(16)	15(13)	-31(13)	16(13)
C18A	195(17)	121(16)	108(16)	17(13)	-29(13)	3(13)
C19A	184(18)	194(18)	280(20)	-38(15)	-22(15)	12(15)
C20A	280(20)	196(19)	320(20)	-93(16)	29(17)	36(16)
C21A	320(20)	154(18)	195(18)	-38(14)	-32(15)	-33(15)
C22A	213(19)	189(18)	178(18)	15(14)	-54(15)	-27(15)
C23A	207(18)	154(17)	170(18)	14(14)	-36(14)	29(14)
C24A	189(17)	97(16)	152(17)	-8(13)	-29(13)	-35(13)
C25A	190(18)	257(19)	207(19)	0(15)	-38(15)	3(15)
C26A	240(20)	340(20)	206(19)	17(16)	-95(16)	-26(16)
C27A	340(20)	216(19)	149(18)	-36(15)	-21(16)	-83(16)
C28A	238(19)	148(17)	227(19)	-40(14)	14(15)	17(15)
C29A	216(19)	165(17)	178(18)	12(14)	-43(15)	24(14)
C30A	176(17)	112(16)	184(18)	-15(13)	-41(14)	5(13)
C31A	129(17)	201(18)	290(20)	-30(15)	-31(15)	-43(14)
C32A	155(17)	123(17)	218(19)	-7(14)	34(14)	-34(13)
C33A	134(16)	137(16)	130(17)	-34(13)	-15(13)	-11(13)
C34A	198(18)	146(17)	216(18)	-8(14)	-90(15)	28(14)
C35A	236(19)	158(17)	138(17)	-4(14)	-73(15)	-20(14)
C36A	172(17)	100(16)	215(18)	-21(14)	-33(14)	-4(13)

C37A	235(19)	125(17)	260(20)	-91(15)	-6(15)	23(14)
C38A	188(18)	186(18)	171(18)	-39(14)	-4(14)	34(14)
C39A	120(16)	154(16)	92(15)	-46(13)	-20(12)	18(13)
C40A	150(17)	135(17)	180(17)	-7(13)	-25(14)	-10(13)
C41A	201(18)	126(17)	280(20)	-2(15)	-50(15)	30(14)
C42A	125(17)	241(19)	330(20)	-49(16)	-17(15)	30(15)
C43A	151(18)	202(19)	260(20)	-44(15)	22(15)	-44(14)
C44A	162(17)	109(16)	183(17)	-22(13)	-12(14)	-2(13)
C45A	159(17)	121(16)	147(16)	-31(13)	-44(13)	-23(13)
C46A	174(18)	168(17)	199(18)	-36(14)	-24(14)	-2(14)
C47A	270(20)	215(19)	151(18)	-33(15)	-4(15)	-92(15)
C48A	340(20)	163(18)	163(18)	26(14)	-118(16)	-110(15)
C49A	241(19)	129(17)	290(20)	-6(15)	-121(16)	4(14)
C50A	181(18)	129(16)	183(18)	-29(14)	-44(14)	-38(13)
C51A	63(15)	114(16)	206(17)	-17(13)	-6(13)	-5(12)
C52A	129(17)	175(18)	169(17)	-29(14)	-8(14)	-26(13)
C53A	192(18)	190(18)	250(20)	-112(15)	-19(15)	-30(14)
C54A	171(18)	93(16)	350(20)	-21(15)	10(15)	-12(14)
C55A	128(17)	184(18)	211(18)	25(15)	13(14)	-20(14)
C56A	137(17)	152(17)	185(18)	-30(14)	-34(14)	11(13)

Ru1B	85(1)	78(1)	142(1)	-19(1)	-24(1)	-2(1)
P1B	108(4)	80(4)	144(4)	-22(3)	-39(3)	1(3)
O1B	91(11)	103(11)	140(11)	-20(9)	-24(9)	-3(9)
O2B	104(11)	106(11)	165(11)	-34(9)	-31(9)	6(9)
N1B	96(13)	122(14)	204(15)	-43(11)	-7(11)	-13(11)
N2B	115(14)	167(15)	321(17)	-103(13)	38(12)	-64(11)
N3B	123(14)	149(14)	190(15)	-75(11)	-55(11)	17(11)
N4B	71(13)	209(15)	264(16)	-102(12)	-12(12)	3(11)
N5B	99(13)	106(13)	189(15)	-7(11)	15(11)	-12(10)
N6B	133(14)	126(14)	228(16)	-34(12)	54(12)	-38(11)
B1B	140(20)	170(20)	310(20)	-91(17)	30(17)	-57(16)
C1B	104(15)	118(16)	114(16)	10(12)	-26(12)	35(12)
C2B	93(16)	124(16)	133(16)	-12(13)	-35(13)	16(13)
C3B	88(16)	150(17)	179(17)	-70(13)	-30(13)	13(13)
C4B	230(18)	72(15)	198(18)	-50(13)	-81(14)	18(13)
C5B	350(20)	630(30)	220(20)	-30(20)	-54(18)	-180(20)
C6B	740(40)	750(40)	260(30)	-10(20)	110(20)	-240(30)
C7B	980(40)	240(20)	190(20)	-1(17)	-280(30)	-80(20)
C8B	580(30)	290(20)	360(30)	-102(19)	-270(20)	90(20)
C9B	320(20)	320(20)	280(20)	-110(17)	-130(17)	49(18)
C10B	147(16)	168(17)	122(16)	-63(13)	-53(13)	-38(13)
C11B	177(18)	129(17)	189(18)	-35(14)	-37(14)	-39(14)
C12B	280(20)	144(17)	195(18)	-26(14)	-92(15)	-22(15)
C13B	360(20)	166(18)	230(20)	13(15)	-107(17)	-119(16)
C14B	270(20)	310(20)	220(20)	2(16)	33(16)	-160(17)
C15B	240(20)	223(19)	203(19)	-67(15)	4(15)	-25(15)
C16B	123(16)	128(16)	64(15)	10(12)	8(12)	7(13)
C17B	116(16)	110(16)	164(17)	-30(13)	-44(13)	23(13)
C18B	79(16)	199(17)	168(17)	5(14)	-8(13)	52(13)
C19B	236(19)	183(18)	228(19)	5(15)	35(15)	107(15)
C20B	330(20)	290(20)	240(20)	105(17)	90(17)	120(17)
C21B	280(20)	470(30)	210(20)	66(19)	19(17)	151(19)
C22B	230(20)	470(30)	185(19)	-112(18)	-54(16)	81(18)
C23B	151(18)	290(20)	179(18)	-27(15)	-57(14)	8(15)
C24B	116(16)	133(16)	114(16)	-58(13)	-13(13)	22(12)
C25B	173(17)	137(17)	169(17)	-31(14)	-40(14)	6(14)
C26B	132(17)	193(18)	270(20)	-86(15)	-78(15)	15(14)
C27B	169(18)	202(18)	245(19)	-90(15)	24(15)	-44(14)
C28B	224(19)	181(18)	176(18)	-15(14)	0(15)	-24(15)
C29B	135(17)	224(18)	168(17)	-16(14)	-30(14)	8(14)
C30B	162(18)	143(17)	252(19)	-32(14)	-40(15)	-19(14)
C31B	280(20)	210(20)	440(20)	-185(18)	21(18)	-115(17)
C32B	177(19)	290(20)	550(30)	-237(19)	86(18)	-137(17)
C33B	238(19)	155(17)	155(17)	-53(14)	-98(15)	73(14)
C34B	240(20)	270(20)	260(20)	-157(16)	-161(16)	160(16)
C35B	120(17)	330(20)	300(20)	-180(17)	-77(15)	54(16)
C36B	193(18)	168(18)	178(18)	-1(14)	-24(15)	14(14)
C37B	300(20)	228(19)	145(18)	22(15)	-8(16)	22(16)
C38B	230(20)	162(18)	230(20)	-10(15)	102(16)	-16(15)
C39B	95(15)	107(16)	176(17)	2(13)	-26(13)	24(12)
C40B	140(17)	166(17)	176(18)	-16(14)	-37(14)	0(13)
C41B	212(18)	191(18)	201(19)	71(15)	-73(15)	-1(14)
C42B	310(20)	102(17)	320(20)	32(15)	-86(17)	-23(15)
C43B	370(20)	125(18)	260(20)	-8(15)	-112(17)	-51(15)

C44B	310(20)	140(17)	171(18)	6(14)	-88(15)	-13(15)
C45B	108(16)	112(16)	135(16)	-7(12)	-58(13)	11(12)
C46B	184(17)	119(16)	154(17)	15(13)	-60(14)	-14(13)
C47B	157(17)	177(18)	160(17)	22(14)	-14(14)	-57(14)
C48B	137(17)	191(17)	140(17)	-32(13)	-37(13)	16(14)
C49B	192(18)	100(16)	178(17)	-20(13)	-56(14)	18(13)
C50B	150(17)	130(16)	149(17)	-18(13)	-29(13)	-38(13)
C51B	176(17)	72(15)	160(17)	7(13)	-54(13)	-12(13)
C52B	174(17)	146(17)	187(18)	-6(13)	-48(14)	-30(14)
C53B	320(20)	212(19)	156(18)	-44(15)	-43(16)	-47(16)
C54B	270(20)	270(20)	240(20)	-31(16)	-121(16)	-101(16)
C55B	150(18)	300(20)	280(20)	-41(16)	-64(16)	-18(15)
C56B	194(18)	199(18)	199(18)	-58(15)	-58(15)	27(14)

Ru1C	108(1)	74(1)	118(1)	-14(1)	-9(1)	-4(1)
P1C	107(4)	90(4)	121(4)	-14(3)	-11(3)	-6(3)
O1C	131(11)	93(11)	131(11)	1(9)	-26(9)	-11(9)
O2C	114(11)	86(11)	175(12)	-21(9)	-26(9)	13(8)
N1C	122(13)	110(13)	143(14)	-17(11)	-19(11)	-1(11)
N2C	140(14)	127(14)	186(14)	-16(11)	-10(11)	-36(11)
N3C	119(13)	123(14)	137(14)	-21(11)	-3(11)	-34(11)
N4C	111(13)	126(14)	180(14)	-40(11)	-6(11)	-17(11)
N5C	125(14)	97(13)	146(14)	-19(11)	17(11)	-5(10)
N6C	134(14)	142(14)	161(14)	-12(11)	43(11)	-26(11)
B1C	160(20)	148(19)	210(20)	-41(16)	26(16)	-23(15)
C1C	94(15)	98(15)	102(15)	25(12)	6(12)	4(12)
C2C	135(17)	86(16)	179(17)	-9(13)	-26(14)	15(13)
C3C	162(17)	99(16)	199(18)	-12(13)	-54(14)	16(13)
C4C	310(20)	124(17)	209(18)	2(14)	-118(16)	-17(14)
C5C	213(19)	168(18)	206(19)	-39(14)	-45(15)	8(14)
C6C	430(20)	220(20)	200(20)	-3(16)	-22(17)	19(17)
C7C	1250(50)	340(30)	210(20)	18(19)	-270(30)	-210(30)
C8C	1900(70)	550(30)	360(30)	170(20)	-510(40)	-780(40)
C9C	1250(50)	450(30)	260(20)	180(20)	-350(30)	-580(30)
C10C	172(17)	85(15)	137(16)	-39(12)	-60(13)	-16(13)
C11C	179(18)	147(17)	249(19)	-22(14)	-49(15)	-15(14)
C12C	240(19)	131(17)	360(20)	-33(15)	-138(17)	24(15)
C13C	360(20)	147(18)	300(20)	67(16)	-160(17)	-66(16)
C14C	290(20)	280(20)	210(20)	25(16)	-30(16)	-122(17)
C15C	171(18)	180(18)	219(19)	-26(14)	-37(15)	-24(14)
C16C	148(16)	108(16)	85(15)	-5(12)	-6(13)	-3(13)
C17C	169(17)	70(15)	182(17)	-17(13)	-43(13)	7(13)
C18C	117(16)	181(17)	185(17)	-2(14)	-35(13)	41(13)
C19C	195(18)	182(18)	237(19)	25(15)	-34(15)	42(14)
C20C	270(20)	250(20)	280(20)	115(17)	-19(17)	27(16)
C21C	340(20)	390(20)	177(19)	34(18)	-47(17)	96(18)
C22C	310(20)	290(20)	200(20)	-73(16)	-53(16)	84(17)
C23C	193(18)	177(18)	201(18)	14(14)	-44(14)	36(14)
C24C	145(16)	96(15)	155(16)	-52(13)	-24(13)	12(12)
C25C	206(18)	153(17)	193(18)	-14(14)	-30(15)	28(14)
C26C	134(17)	194(18)	260(19)	-68(15)	-58(15)	25(14)
C27C	156(18)	167(18)	231(19)	-94(14)	17(14)	-45(14)
C28C	200(18)	152(17)	156(17)	-11(14)	-10(14)	-10(14)
C29C	158(17)	129(16)	183(18)	-32(13)	-36(14)	22(13)
C30C	191(18)	136(17)	133(17)	-27(13)	-27(14)	18(14)
C31C	280(20)	131(17)	270(20)	-64(15)	-74(16)	-53(15)
C32C	213(19)	131(17)	290(20)	-44(15)	-22(16)	-75(14)
C33C	153(17)	115(16)	159(17)	-11(13)	-45(14)	-10(13)
C34C	156(17)	132(17)	212(18)	-43(14)	-50(14)	41(13)
C35C	92(16)	203(18)	207(18)	-70(14)	0(14)	5(14)
C36C	163(18)	195(18)	181(18)	-34(14)	-22(14)	24(14)
C37C	300(20)	290(20)	124(18)	50(15)	-17(16)	36(16)
C38C	221(19)	212(19)	182(18)	27(14)	53(15)	-12(15)
C39C	84(15)	98(15)	152(16)	-13(13)	18(13)	4(12)
C40C	150(17)	163(17)	176(18)	-28(14)	-35(14)	-19(13)
C41C	178(18)	199(18)	211(18)	28(15)	-60(15)	40(14)
C42C	199(18)	89(16)	202(18)	15(14)	22(14)	25(14)
C43C	179(18)	146(17)	151(17)	-37(14)	33(14)	-43(14)

C44C	153(17)	133(16)	124(16)	-7(13)	-14(13)	-5(13)
C45C	121(16)	156(16)	122(16)	-32(13)	-35(13)	-2(13)
C46C	184(18)	122(17)	178(17)	4(14)	-9(14)	2(14)
C47C	198(19)	199(19)	215(19)	-8(15)	54(15)	-44(15)
C48C	143(17)	260(20)	202(18)	-66(15)	39(14)	31(15)
C49C	195(18)	137(17)	166(17)	-33(14)	-34(14)	48(14)
C50C	147(17)	136(16)	116(16)	-34(13)	-31(13)	-23(13)
C51C	173(17)	71(15)	148(16)	35(12)	-46(13)	-8(13)
C52C	149(17)	141(16)	126(16)	24(13)	-26(13)	-3(13)
C53C	246(19)	123(17)	152(17)	-14(13)	-53(14)	-21(14)
C54C	212(18)	151(17)	209(18)	3(14)	-89(15)	-81(14)
C55C	156(17)	199(18)	195(18)	26(14)	-22(14)	-36(14)
C56C	162(17)	152(17)	155(17)	-37(14)	-36(14)	3(13)

C1	490(20)	2710(80)	1090(50)	-1230(50)	40(30)	-190(40)
C2	490(20)	2710(80)	1090(50)	-1230(50)	40(30)	-190(40)
C3	490(20)	2710(80)	1090(50)	-1230(50)	40(30)	-190(40)
C4	490(20)	2710(80)	1090(50)	-1230(50)	40(30)	-190(40)
C5	490(20)	2710(80)	1090(50)	-1230(50)	40(30)	-190(40)
C6	490(20)	2710(80)	1090(50)	-1230(50)	40(30)	-190(40)
C7	490(20)	2710(80)	1090(50)	-1230(50)	40(30)	-190(40)
C9	530(30)	700(40)	2180(80)	-990(50)	640(40)	-430(30)
C10	540(40)	1320(60)	700(40)	20(40)	50(30)	220(40)
C11	440(30)	1240(50)	660(40)	380(40)	-10(30)	150(30)
C12	660(40)	530(30)	590(30)	40(30)	-50(30)	190(30)
C13	1500(70)	810(50)	760(40)	-100(40)	-480(40)	-20(40)

Table 11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 2 CCDC 164301 MSS14.

	x	y	z	U_{iso}
H1A	130(20)	163(14)	3296(12)	18
H2A	3690(20)	1030(15)	1828(12)	18
H3A	3860(20)	2159(15)	1124(13)	21
H5A	3500(20)	1741(17)	2480(13)	32
H6A	3660(30)	2358(17)	3180(15)	42
H7A	4250(30)	3413(17)	2955(15)	42
H8A	4770(30)	3690(18)	2023(15)	44
H9A	4740(20)	3075(16)	1332(14)	35
H11A	5700(20)	1637(15)	1828(13)	25
H12A	7260(20)	1327(16)	1466(14)	31
H13A	7660(30)	1242(16)	573(14)	36
H14A	6450(20)	1463(16)	22(14)	32
H15A	4870(20)	1749(15)	397(13)	28
H17A	550(20)	2291(14)	615(12)	16
H19A	160(20)	3251(15)	971(13)	26
H20A	570(30)	4214(17)	1184(14)	33
H21A	2180(20)	4498(16)	1067(13)	27
H22A	3380(20)	3805(15)	736(13)	23
H23A	2960(20)	2840(15)	494(13)	22
H25A	380(20)	2584(15)	-248(13)	26
H26A	900(20)	2527(16)	-1187(14)	31
H27A	2460(20)	2093(16)	-1486(14)	28
H28A	3430(20)	1790(15)	-896(13)	25
H29A	2880(20)	1819(15)	31(13)	23
H30A	-600(20)	190(14)	1325(13)	19
H31A	-1990(20)	-162(15)	2036(13)	25
H32A	-1440(20)	-158(15)	2940(13)	21
H33A	3380(20)	-131(14)	2013(12)	16
H34A	3320(20)	-722(15)	2933(13)	22
H35A	1640(20)	-509(15)	3407(13)	21
H36A	1420(20)	2170(15)	2083(13)	19
H37A	720(20)	2398(16)	3030(13)	25
H38A	140(20)	1362(15)	3489(13)	22
H40A	3130(20)	-1194(15)	1241(12)	19
H41A	4730(20)	-1439(16)	1167(13)	24
H42A	5890(20)	-690(15)	819(13)	28
H43A	5370(20)	330(16)	542(13)	25
H44A	3770(20)	578(15)	642(12)	18
H46A	2980(20)	-146(15)	-78(13)	22
H47A	2610(20)	158(15)	-914(13)	25
H48A	1200(20)	730(15)	-997(13)	25
H49A	160(20)	953(15)	-252(13)	25
H50A	470(20)	624(14)	608(13)	19
H52A	1600(20)	-1037(15)	457(13)	19
H53A	1320(20)	-2076(15)	595(13)	25
H54A	990(20)	-2527(16)	1467(13)	25
H55A	940(20)	-1901(15)	2163(13)	22
H56A	1240(20)	-849(15)	2020(12)	19

H1B	7350(20)	2755(15)	5061(12)	25
H2B	4410(20)	856(14)	5414(12)	14
H3B	2450(20)	949(14)	5389(12)	16
H5B	4480(30)	995(18)	4429(15)	47
H6B	4470(30)	1040(20)	3552(19)	72
H7B	3160(30)	921(19)	3169(17)	54
H8B	1710(30)	690(18)	3738(15)	46
H9B	1750(30)	641(17)	4669(14)	35
H11B	4130(20)	-267(14)	4980(12)	19
H12B	4070(20)	-1322(15)	5344(13)	24
H13B	2860(20)	-1636(16)	6054(13)	29
H14B	1660(20)	-867(16)	6415(14)	32
H15B	1800(20)	149(16)	6019(13)	27
H17B	1760(20)	3197(14)	5900(12)	15
H19B	2340(20)	3858(16)	5114(13)	28
H20B	2680(30)	4055(17)	4166(14)	38
H21B	2430(30)	3301(17)	3629(15)	41
H22B	1930(20)	2309(17)	3987(14)	35
H23B	1570(20)	2120(16)	4912(13)	24
H25B	0(20)	3015(15)	5524(13)	19
H26B	-1430(20)	2569(15)	5848(13)	23
H27B	-1560(20)	1710(15)	6498(13)	25
H28B	-150(20)	1379(16)	6839(13)	24
H29B	1350(20)	1837(15)	6486(12)	21
H30B	4790(20)	3434(15)	6681(13)	22
H31B	6230(30)	4132(18)	6414(15)	37
H32B	7270(30)	3668(18)	5702(15)	41
H33B	5660(20)	777(15)	6152(13)	21
H34B	7390(20)	565(16)	5797(13)	29
H35B	7970(20)	1616(16)	5330(14)	28
H36B	3860(20)	2468(15)	4747(13)	22
H37B	4960(20)	2796(16)	3886(14)	28
H38B	6570(20)	2891(16)	4177(13)	27
H40B	4770(20)	1052(15)	7770(13)	19
H41B	4660(20)	-14(15)	8089(13)	24
H42B	4100(20)	-682(16)	7558(13)	29
H43B	3620(20)	-351(16)	6761(13)	30
H44B	3740(20)	714(15)	6464(13)	24
H46B	2470(20)	1204(15)	7426(12)	18
H47B	970(20)	1548(15)	7810(12)	20
H48B	520(20)	2602(14)	7791(12)	18
H49B	1690(20)	3333(15)	7398(12)	18
H50B	3200(20)	3016(15)	6989(12)	17
H52B	3980(20)	2475(15)	7857(12)	20
H53B	5030(20)	2788(16)	8371(14)	27
H54B	6650(20)	2724(16)	8105(14)	30
H55B	7250(20)	2291(16)	7305(13)	29
H56B	6230(20)	1971(15)	6757(13)	23

H1C	12200(20)	5474(14)	1762(12)	21
H2C	9200(20)	3622(14)	2088(12)	16
H3C	7200(20)	3670(15)	2082(12)	18
H5C	8730(20)	4185(15)	1135(13)	23
H6C	8910(20)	4196(17)	195(14)	35
H7C	7970(30)	3490(20)	-156(18)	70
H8C	6910(40)	2800(30)	430(20)	106
H9C	6870(30)	2780(20)	1376(18)	75
H11C	9090(20)	2511(15)	1878(13)	23
H12C	9070(20)	1464(16)	2201(13)	28
H13C	7610(20)	1090(17)	2744(13)	31
H14C	6330(30)	1779(16)	2946(14)	31
H15C	6350(20)	2828(15)	2580(12)	23
H17C	6470(20)	5953(15)	2488(12)	17
H19C	7000(20)	6574(15)	1693(13)	25
H20C	7350(30)	6627(17)	747(14)	34
H21C	7230(30)	5783(17)	242(15)	37
H22C	6720(20)	4850(16)	698(14)	32
H23C	6380(20)	4724(15)	1651(13)	23
H25C	4740(20)	5708(15)	2104(13)	22
H26C	3290(20)	5243(15)	2508(13)	23
H27C	3210(20)	4509(15)	3231(13)	22
H28C	4650(20)	4248(15)	3637(13)	21
H29C	6040(20)	4690(15)	3218(12)	19
H30C	9500(20)	6248(14)	3306(12)	18
H31C	10960(20)	6931(16)	3114(13)	26
H32C	12110(20)	6409(15)	2399(13)	25
H33C	10300(20)	3552(15)	2799(12)	17
H34C	12080(20)	3264(15)	2520(12)	20
H35C	12720(20)	4281(15)	2081(13)	20
H36C	8620(20)	5394(15)	1407(12)	22
H37C	9790(20)	5797(16)	593(14)	30
H38C	11460(20)	5782(15)	890(13)	26
H40C	9800(20)	3794(15)	4281(12)	19
H41C	9810(20)	2721(15)	4561(13)	24
H42C	8930(20)	2059(15)	4149(12)	21
H43C	8180(20)	2463(15)	3430(12)	20
H44C	8190(20)	3525(14)	3183(12)	17
H46C	7330(20)	3988(15)	4221(12)	20
H47C	5840(20)	4298(16)	4630(13)	26
H48C	5280(20)	5357(15)	4525(13)	25
H49C	6310(20)	6083(15)	4017(12)	20
H50C	7810(20)	5769(14)	3550(12)	16
H52C	8700(20)	5310(14)	4458(12)	17
H53C	9670(20)	5832(15)	4909(13)	20
H54C	11320(20)	5806(15)	4624(12)	22
H55C	11990(20)	5217(15)	3901(12)	22
H56C	10940(20)	4717(15)	3446(13)	18

H1	9750	10140	4268	165
H2	9588	11185	4465	165
H3	9787	11450	5305	165
H4	10148	10671	5948	165
H5	10309	9626	5751	165
H7D	10076	9012	4544	165
H7E	9703	8839	5159	165
H7F	10803	8927	4948	165
H9D	4065	4894	1219	141
H9E	4779	4892	671	141
H9F	3678	5021	675	141
H10A	3772	6003	1057	107
H10B	4872	5874	1052	107
H11D	4009	6117	158	99
H11E	5099	5923	128	99
H12D	5335	6893	559	74
H12E	5020	7064	-3	74
H13D	4077	7660	645	119
H13E	3727	7037	991	119
H13F	3414	7209	430	119

Table 12. Torsion angles [°] for 2 CCDC 164301 MSS14.

C1A-Ru1A-P1A-C45A	-78.97(14)	N1A-Ru1A-N5A-C36A	-140.6(3)
N3A-Ru1A-P1A-C45A	-176.68(13)	P1A-Ru1A-N5A-C36A	150.8(9)
O1A-Ru1A-P1A-C45A	1.93(12)	C1A-Ru1A-N5A-N6A	-144.2(2)
N5A-Ru1A-P1A-C45A	162.3(10)	N3A-Ru1A-N5A-N6A	-46.3(2)
N1A-Ru1A-P1A-C45A	94.01(13)	O1A-Ru1A-N5A-N6A	135.3(2)
C1A-Ru1A-P1A-C39A	43.25(14)	N1A-Ru1A-N5A-N6A	43.4(2)
N3A-Ru1A-P1A-C39A	-54.46(13)	P1A-Ru1A-N5A-N6A	-25.2(12)
O1A-Ru1A-P1A-C39A	124.14(12)	C36A-N5A-N6A-C38A	0.6(3)
N5A-Ru1A-P1A-C39A	-75.5(11)	Ru1A-N5A-N6A-C38A	177.7(2)
N1A-Ru1A-P1A-C39A	-143.78(13)	C36A-N5A-N6A-B1A	-176.5(3)
C1A-Ru1A-P1A-C51A	158.46(14)	Ru1A-N5A-N6A-B1A	0.6(3)
N3A-Ru1A-P1A-C51A	60.75(13)	C32A-N2A-B1A-N4A	131.6(3)
O1A-Ru1A-P1A-C51A	-120.65(12)	N1A-N2A-B1A-N4A	-57.2(3)
N5A-Ru1A-P1A-C51A	39.7(11)	C32A-N2A-B1A-N6A	-111.4(3)
N1A-Ru1A-P1A-C51A	-28.57(13)	N1A-N2A-B1A-N6A	59.7(3)
C1A-Ru1A-O1A-C16A	2.4(2)	C35A-N4A-B1A-N2A	-127.1(3)
N3A-Ru1A-O1A-C16A	78.9(6)	N3A-N4A-B1A-N2A	63.6(3)
N5A-Ru1A-O1A-C16A	89.8(2)	C35A-N4A-B1A-N6A	115.3(3)
N1A-Ru1A-O1A-C16A	174.7(2)	N3A-N4A-B1A-N6A	-54.0(3)
P1A-Ru1A-O1A-C16A	-91.5(2)	C38A-N6A-B1A-N2A	122.1(3)
C1A-Ru1A-N1A-C30A	83.6(6)	N5A-N6A-B1A-N2A	-61.5(3)
N3A-Ru1A-N1A-C30A	-148.4(3)	C38A-N6A-B1A-N4A	-119.3(3)
O1A-Ru1A-N1A-C30A	39.9(3)	N5A-N6A-B1A-N4A	57.0(3)
N5A-Ru1A-N1A-C30A	127.1(3)	C16A-O2A-C1A-C2A	-166.2(3)
P1A-Ru1A-N1A-C30A	-56.5(3)	C16A-O2A-C1A-Ru1A	5.4(3)
C1A-Ru1A-N1A-N2A	-88.0(6)	N3A-Ru1A-C1A-C2A	-8.4(4)
N3A-Ru1A-N1A-N2A	39.9(2)	O1A-Ru1A-C1A-C2A	163.4(4)
O1A-Ru1A-N1A-N2A	-131.7(2)	N5A-Ru1A-C1A-C2A	75.6(4)
N5A-Ru1A-N1A-N2A	-44.6(2)	N1A-Ru1A-C1A-C2A	118.9(6)
P1A-Ru1A-N1A-N2A	131.87(19)	P1A-Ru1A-C1A-C2A	-101.1(4)
C30A-N1A-N2A-C32A	-0.1(3)	N3A-Ru1A-C1A-O2A	-175.67(17)
Ru1A-N1A-N2A-C32A	173.77(19)	O1A-Ru1A-C1A-O2A	-3.89(16)
C30A-N1A-N2A-B1A	-173.1(3)	N5A-Ru1A-C1A-O2A	-91.66(18)
Ru1A-N1A-N2A-B1A	0.8(3)	N1A-Ru1A-C1A-O2A	-48.3(7)
C1A-Ru1A-N3A-C33A	-43.1(3)	P1A-Ru1A-C1A-O2A	91.70(17)
O1A-Ru1A-N3A-C33A	-118.4(6)	O2A-C1A-C2A-C3A	4.6(4)
N5A-Ru1A-N3A-C33A	-129.4(3)	Ru1A-C1A-C2A-C3A	-162.7(3)
N1A-Ru1A-N3A-C33A	145.6(3)	C1A-C2A-C3A-C10A	-126.2(4)
P1A-Ru1A-N3A-C33A	52.0(3)	C1A-C2A-C3A-C4A	109.2(4)
C1A-Ru1A-N3A-N4A	135.8(2)	C2A-C3A-C4A-C5A	15.7(4)
O1A-Ru1A-N3A-N4A	60.4(7)	C10A-C3A-C4A-C5A	-109.2(3)
N5A-Ru1A-N3A-N4A	49.5(2)	C2A-C3A-C4A-C9A	-166.7(3)
N1A-Ru1A-N3A-N4A	-35.5(2)	C10A-C3A-C4A-C9A	68.4(4)
P1A-Ru1A-N3A-N4A	-129.15(19)	C9A-C4A-C5A-C6A	-1.8(5)
C33A-N3A-N4A-C35A	0.2(3)	C3A-C4A-C5A-C6A	175.8(3)
Ru1A-N3A-N4A-C35A	-179.00(19)	C4A-C5A-C6A-C7A	1.4(6)
C33A-N3A-N4A-B1A	171.5(3)	C5A-C6A-C7A-C8A	0.1(6)
Ru1A-N3A-N4A-B1A	-7.7(3)	C6A-C7A-C8A-C9A	-1.1(6)
C1A-Ru1A-N5A-C36A	31.9(3)	C5A-C4A-C9A-C8A	0.7(5)
N3A-Ru1A-N5A-C36A	129.7(3)	C3A-C4A-C9A-C8A	-176.9(3)
O1A-Ru1A-N5A-C36A	-48.7(3)	C7A-C8A-C9A-C4A	0.7(5)

C2A-C3A-C10A-C11A	-88.5(4)
C4A-C3A-C10A-C11A	37.3(4)
C2A-C3A-C10A-C15A	91.6(4)
C4A-C3A-C10A-C15A	-142.7(3)
C15A-C10A-C11A-C12A	-0.3(5)
C3A-C10A-C11A-C12A	179.8(3)
C10A-C11A-C12A-C13A	0.3(5)
C11A-C12A-C13A-C14A	0.0(5)
C12A-C13A-C14A-C15A	-0.4(5)
C13A-C14A-C15A-C10A	0.4(5)
C11A-C10A-C15A-C14A	-0.1(5)
C3A-C10A-C15A-C14A	179.9(3)
Ru1A-O1A-C16A-O2A	0.3(4)
Ru1A-O1A-C16A-C17A	-178.6(2)
C1A-O2A-C16A-O1A	-4.0(4)
C1A-O2A-C16A-C17A	175.0(2)
O1A-C16A-C17A-C18A	129.0(3)
O2A-C16A-C17A-C18A	-50.1(4)
O1A-C16A-C17A-C24A	-103.8(3)
O2A-C16A-C17A-C24A	77.1(3)
C16A-C17A-C18A-C19A	-109.1(3)
C24A-C17A-C18A-C19A	123.0(3)
C16A-C17A-C18A-C23A	71.6(4)
C24A-C17A-C18A-C23A	-56.3(4)
C23A-C18A-C19A-C20A	1.3(5)
C17A-C18A-C19A-C20A	-178.1(3)
C18A-C19A-C20A-C21A	-0.9(5)
C19A-C20A-C21A-C22A	-0.4(5)
C20A-C21A-C22A-C23A	1.3(5)
C21A-C22A-C23A-C18A	-0.9(5)
C19A-C18A-C23A-C22A	-0.4(5)
C17A-C18A-C23A-C22A	178.9(3)
C16A-C17A-C24A-C25A	143.7(3)
C18A-C17A-C24A-C25A	-88.9(3)
C16A-C17A-C24A-C29A	-40.4(4)
C18A-C17A-C24A-C29A	87.0(4)
C29A-C24A-C25A-C26A	0.3(5)
C17A-C24A-C25A-C26A	176.4(3)
C24A-C25A-C26A-C27A	-0.4(5)
C25A-C26A-C27A-C28A	0.2(5)
C26A-C27A-C28A-C29A	0.0(5)
C27A-C28A-C29A-C24A	-0.1(5)
C25A-C24A-C29A-C28A	-0.1(5)
C17A-C24A-C29A-C28A	-175.9(3)
N2A-N1A-C30A-C31A	0.1(3)
Ru1A-N1A-C30A-C31A	-172.3(2)
N1A-C30A-C31A-C32A	0.0(4)
N1A-N2A-C32A-C31A	0.1(3)
B1A-N2A-C32A-C31A	171.8(3)
C30A-C31A-C32A-N2A	-0.1(4)
N4A-N3A-C33A-C34A	0.2(3)
Ru1A-N3A-C33A-C34A	179.1(2)
N3A-C33A-C34A-C35A	-0.4(4)
N3A-N4A-C35A-C34A	-0.5(3)
B1A-N4A-C35A-C34A	-170.8(3)
C33A-C34A-C35A-N4A	0.5(4)
N6A-N5A-C36A-C37A	-0.5(3)
Ru1A-N5A-C36A-C37A	-176.9(2)
N5A-C36A-C37A-C38A	0.2(4)
N5A-N6A-C38A-C37A	-0.4(4)
B1A-N6A-C38A-C37A	176.2(3)
C36A-C37A-C38A-N6A	0.1(4)
C45A-P1A-C39A-C40A	-120.0(3)
C51A-P1A-C39A-C40A	-15.5(3)
Ru1A-P1A-C39A-C40A	110.5(2)
C45A-P1A-C39A-C44A	64.0(3)
C51A-P1A-C39A-C44A	168.5(2)
Ru1A-P1A-C39A-C44A	-65.5(3)
C44A-C39A-C40A-C41A	0.4(5)
P1A-C39A-C40A-C41A	-175.6(2)
C39A-C40A-C41A-C42A	-0.3(5)
C40A-C41A-C42A-C43A	0.0(5)
C41A-C42A-C43A-C44A	0.3(5)
C42A-C43A-C44A-C39A	-0.3(5)
C40A-C39A-C44A-C43A	-0.1(5)
P1A-C39A-C44A-C43A	176.1(2)
C39A-P1A-C45A-C46A	13.2(3)
C51A-P1A-C45A-C46A	-87.6(3)
Ru1A-P1A-C45A-C46A	142.2(2)
C39A-P1A-C45A-C50A	-168.3(2)
C51A-P1A-C45A-C50A	91.0(3)
Ru1A-P1A-C45A-C50A	-39.2(3)
C50A-C45A-C46A-C47A	1.1(5)
P1A-C45A-C46A-C47A	179.7(2)
C45A-C46A-C47A-C48A	0.4(5)
C46A-C47A-C48A-C49A	-1.5(5)
C47A-C48A-C49A-C50A	1.1(5)
C48A-C49A-C50A-C45A	0.4(5)
C46A-C45A-C50A-C49A	-1.5(4)
P1A-C45A-C50A-C49A	179.8(2)
C45A-P1A-C51A-C52A	29.8(3)
C39A-P1A-C51A-C52A	-75.1(3)
Ru1A-P1A-C51A-C52A	159.7(2)
C45A-P1A-C51A-C56A	-162.8(2)
C39A-P1A-C51A-C56A	92.4(3)
Ru1A-P1A-C51A-C56A	-32.9(3)
C56A-C51A-C52A-C53A	-1.3(5)
P1A-C51A-C52A-C53A	166.2(2)
C51A-C52A-C53A-C54A	-0.8(5)
C52A-C53A-C54A-C55A	2.1(5)
C53A-C54A-C55A-C56A	-1.2(5)
C52A-C51A-C56A-C55A	2.3(5)
P1A-C51A-C56A-C55A	-165.5(2)
C54A-C55A-C56A-C51A	-1.0(5)
C1B-Ru1B-P1B-C45B	-72.07(14)
N3B-Ru1B-P1B-C45B	-170.33(12)
O1B-Ru1B-P1B-C45B	8.04(12)
N5B-Ru1B-P1B-C45B	142(4)

N1B-Ru1B-P1B-C45B	102.19(13)
C1B-Ru1B-P1B-C39B	48.77(14)
N3B-Ru1B-P1B-C39B	-49.49(13)
O1B-Ru1B-P1B-C39B	128.87(13)
N5B-Ru1B-P1B-C39B	-97(4)
N1B-Ru1B-P1B-C39B	-136.97(13)
C1B-Ru1B-P1B-C51B	169.72(13)
N3B-Ru1B-P1B-C51B	71.47(13)
O1B-Ru1B-P1B-C51B	-110.17(12)
N5B-Ru1B-P1B-C51B	24(4)
N1B-Ru1B-P1B-C51B	-16.02(12)
C1B-Ru1B-O1B-C16B	1.4(2)
N3B-Ru1B-O1B-C16B	73.4(7)
N5B-Ru1B-O1B-C16B	87.4(2)
N1B-Ru1B-O1B-C16B	172.59(19)
P1B-Ru1B-O1B-C16B	-93.38(19)
C1B-Ru1B-N1B-C30B	99.2(6)
N3B-Ru1B-N1B-C30B	-142.1(3)
O1B-Ru1B-N1B-C30B	44.9(3)
N5B-Ru1B-N1B-C30B	132.1(3)
P1B-Ru1B-N1B-C30B	-48.6(3)
C1B-Ru1B-N1B-N2B	-75.0(6)
N3B-Ru1B-N1B-N2B	43.7(2)
O1B-Ru1B-N1B-N2B	-129.3(2)
N5B-Ru1B-N1B-N2B	-42.1(2)
P1B-Ru1B-N1B-N2B	137.2(2)
C30B-N1B-N2B-C32B	-0.2(4)
Ru1B-N1B-N2B-C32B	175.6(2)
C30B-N1B-N2B-B1B	-177.6(3)
Ru1B-N1B-N2B-B1B	-1.7(4)
C1B-Ru1B-N3B-C33B	-49.2(3)
O1B-Ru1B-N3B-C33B	-120.1(7)
N5B-Ru1B-N3B-C33B	-134.1(3)
N1B-Ru1B-N3B-C33B	140.3(3)
P1B-Ru1B-N3B-C33B	46.7(3)
C1B-Ru1B-N3B-N4B	130.4(2)
O1B-Ru1B-N3B-N4B	59.5(8)
N5B-Ru1B-N3B-N4B	45.4(2)
N1B-Ru1B-N3B-N4B	-40.1(2)
P1B-Ru1B-N3B-N4B	-133.7(2)
C33B-N3B-N4B-C35B	0.1(3)
Ru1B-N3B-N4B-C35B	-179.6(2)
C33B-N3B-N4B-B1B	175.7(3)
Ru1B-N3B-N4B-B1B	-3.9(4)
C1B-Ru1B-N5B-C36B	32.3(3)
N3B-Ru1B-N5B-C36B	130.6(3)
O1B-Ru1B-N5B-C36B	-47.7(3)
N1B-Ru1B-N5B-C36B	-141.8(3)
P1B-Ru1B-N5B-C36B	178(100)
C1B-Ru1B-N5B-N6B	-142.0(2)
N3B-Ru1B-N5B-N6B	-43.8(2)
O1B-Ru1B-N5B-N6B	138.0(2)
N1B-Ru1B-N5B-N6B	43.8(2)
P1B-Ru1B-N5B-N6B	4(4)
C36B-N5B-N6B-C38B	-0.4(3)
Ru1B-N5B-N6B-C38B	175.4(2)
C36B-N5B-N6B-B1B	-176.8(3)
Ru1B-N5B-N6B-B1B	-1.0(3)
C38B-N6B-B1B-N2B	124.6(3)
N5B-N6B-B1B-N2B	-60.0(4)
C38B-N6B-B1B-N4B	-117.6(4)
N5B-N6B-B1B-N4B	57.8(3)
C32B-N2B-B1B-N6B	-115.0(4)
N1B-N2B-B1B-N6B	61.7(4)
C32B-N2B-B1B-N4B	127.4(4)
N1B-N2B-B1B-N4B	-55.9(4)
C35B-N4B-B1B-N6B	117.9(3)
N3B-N4B-B1B-N6B	-56.8(4)
C35B-N4B-B1B-N2B	-123.9(3)
N3B-N4B-B1B-N2B	61.4(4)
C16B-O2B-C1B-C2B	-162.6(3)
C16B-O2B-C1B-Ru1B	7.9(3)
N3B-Ru1B-C1B-C2B	-11.9(4)
O1B-Ru1B-C1B-C2B	161.3(4)
N5B-Ru1B-C1B-C2B	73.0(4)
N1B-Ru1B-C1B-C2B	106.0(6)
P1B-Ru1B-C1B-C2B	-106.3(4)
N3B-Ru1B-C1B-O2B	-177.85(17)
O1B-Ru1B-C1B-O2B	-4.72(16)
N5B-Ru1B-C1B-O2B	-92.96(18)
N1B-Ru1B-C1B-O2B	-60.0(6)
P1B-Ru1B-C1B-O2B	87.66(17)
O2B-C1B-C2B-C3B	-4.0(4)
Ru1B-C1B-C2B-C3B	-170.0(3)
C1B-C2B-C3B-C10B	-126.3(3)
C1B-C2B-C3B-C4B	107.5(4)
C2B-C3B-C4B-C5B	21.2(5)
C10B-C3B-C4B-C5B	-104.3(4)
C2B-C3B-C4B-C9B	-159.6(3)
C10B-C3B-C4B-C9B	74.9(4)
C9B-C4B-C5B-C6B	-1.2(6)
C3B-C4B-C5B-C6B	177.9(4)
C4B-C5B-C6B-C7B	1.2(8)
C5B-C6B-C7B-C8B	-0.6(8)
C6B-C7B-C8B-C9B	0.0(7)
C7B-C8B-C9B-C4B	-0.1(6)
C5B-C4B-C9B-C8B	0.7(5)
C3B-C4B-C9B-C8B	-178.5(3)
C2B-C3B-C10B-C15B	103.9(3)
C4B-C3B-C10B-C15B	-128.1(3)
C2B-C3B-C10B-C11B	-74.7(4)
C4B-C3B-C10B-C11B	53.3(4)
C15B-C10B-C11B-C12B	0.1(5)
C3B-C10B-C11B-C12B	178.7(3)
C10B-C11B-C12B-C13B	-0.2(5)
C11B-C12B-C13B-C14B	0.3(5)
C12B-C13B-C14B-C15B	-0.3(5)
C11B-C10B-C15B-C14B	-0.1(5)

C3B-C10B-C15B-C14B	-178.7(3)
C13B-C14B-C15B-C10B	0.2(5)
Ru1B-O1B-C16B-O2B	3.2(3)
Ru1B-O1B-C16B-C17B	-169.4(2)
C1B-O2B-C16B-O1B	-7.5(4)
C1B-O2B-C16B-C17B	165.4(2)
O1B-C16B-C17B-C24B	-138.3(3)
O2B-C16B-C17B-C24B	48.6(4)
O1B-C16B-C17B-C18B	95.8(3)
O2B-C16B-C17B-C18B	-77.3(3)
C16B-C17B-C18B-C23B	79.6(3)
C24B-C17B-C18B-C23B	-47.3(4)
C16B-C17B-C18B-C19B	-94.8(3)
C24B-C17B-C18B-C19B	138.2(3)
C23B-C18B-C19B-C20B	2.1(5)
C17B-C18B-C19B-C20B	176.7(3)
C18B-C19B-C20B-C21B	-0.9(5)
C19B-C20B-C21B-C22B	-0.9(6)
C20B-C21B-C22B-C23B	1.5(5)
C19B-C18B-C23B-C22B	-1.5(5)
C17B-C18B-C23B-C22B	-175.9(3)
C21B-C22B-C23B-C18B	-0.3(5)
C16B-C17B-C24B-C29B	18.1(4)
C18B-C17B-C24B-C29B	139.1(3)
C16B-C17B-C24B-C25B	-165.9(3)
C18B-C17B-C24B-C25B	-45.0(4)
C29B-C24B-C25B-C26B	-1.5(5)
C17B-C24B-C25B-C26B	-177.7(3)
C24B-C25B-C26B-C27B	0.7(5)
C25B-C26B-C27B-C28B	0.4(5)
C26B-C27B-C28B-C29B	-0.7(5)
C25B-C24B-C29B-C28B	1.2(5)
C17B-C24B-C29B-C28B	177.2(3)
C27B-C28B-C29B-C24B	-0.2(5)
N2B-N1B-C30B-C31B	-0.3(4)
Ru1B-N1B-C30B-C31B	-174.9(3)
N1B-C30B-C31B-C32B	0.7(5)
N1B-N2B-C32B-C31B	0.7(5)
B1B-N2B-C32B-C31B	177.6(4)
C30B-C31B-C32B-N2B	-0.8(5)
N4B-N3B-C33B-C34B	0.1(3)
Ru1B-N3B-C33B-C34B	179.7(2)
N3B-C33B-C34B-C35B	-0.2(4)
C33B-C34B-C35B-N4B	0.3(4)
N3B-N4B-C35B-C34B	-0.2(4)
B1B-N4B-C35B-C34B	-175.4(3)
N6B-N5B-C36B-C37B	0.2(3)
Ru1B-N5B-C36B-C37B	-174.7(2)
N5B-C36B-C37B-C38B	0.1(4)
N5B-N6B-C38B-C37B	0.5(4)
B1B-N6B-C38B-C37B	176.2(3)
C36B-C37B-C38B-N6B	-0.3(4)
C45B-P1B-C39B-C44B	88.4(3)
C51B-P1B-C39B-C44B	-166.7(3)
Ru1B-P1B-C39B-C44B	-39.1(3)
C45B-P1B-C39B-C40B	-87.3(3)
C51B-P1B-C39B-C40B	17.6(3)
Ru1B-P1B-C39B-C40B	145.2(2)
C44B-C39B-C40B-C41B	-0.2(5)
P1B-C39B-C40B-C41B	175.5(2)
C39B-C40B-C41B-C42B	0.7(5)
C40B-C41B-C42B-C43B	-0.4(5)
C41B-C42B-C43B-C44B	-0.3(6)
C42B-C43B-C44B-C39B	0.8(5)
C40B-C39B-C44B-C43B	-0.5(5)
P1B-C39B-C44B-C43B	-176.4(3)
C39B-P1B-C45B-C46B	-10.5(3)
C51B-P1B-C45B-C46B	-113.5(3)
Ru1B-P1B-C45B-C46B	121.7(2)
C39B-P1B-C45B-C50B	170.4(2)
C51B-P1B-C45B-C50B	67.4(3)
Ru1B-P1B-C45B-C50B	-57.4(3)
C50B-C45B-C46B-C47B	1.3(5)
P1B-C45B-C46B-C47B	-177.9(2)
C45B-C46B-C47B-C48B	-1.4(5)
C46B-C47B-C48B-C49B	0.0(5)
C47B-C48B-C49B-C50B	1.5(5)
C48B-C49B-C50B-C45B	-1.7(5)
C46B-C45B-C50B-C49B	0.3(4)
P1B-C45B-C50B-C49B	179.4(2)
C45B-P1B-C51B-C52B	7.5(3)
C39B-P1B-C51B-C52B	-95.4(3)
Ru1B-P1B-C51B-C52B	132.3(2)
C45B-P1B-C51B-C56B	-173.8(2)
C39B-P1B-C51B-C56B	83.3(3)
Ru1B-P1B-C51B-C56B	-49.0(3)
C56B-C51B-C52B-C53B	-0.2(5)
P1B-C51B-C52B-C53B	178.5(2)
C51B-C52B-C53B-C54B	-1.4(5)
C52B-C53B-C54B-C55B	1.6(5)
C53B-C54B-C55B-C56B	-0.3(5)
C54B-C55B-C56B-C51B	-1.3(5)
C52B-C51B-C56B-C55B	1.5(5)
P1B-C51B-C56B-C55B	-177.2(3)
C1C-Ru1C-P1C-C39C	49.91(14)
N3C-Ru1C-P1C-C39C	-46.86(13)
O1C-Ru1C-P1C-C39C	129.64(12)
N5C-Ru1C-P1C-C39C	-113.8(13)
N1C-Ru1C-P1C-C39C	-135.21(13)
C1C-Ru1C-P1C-C45C	-72.16(14)
N3C-Ru1C-P1C-C45C	-168.92(13)
O1C-Ru1C-P1C-C45C	7.58(12)
N5C-Ru1C-P1C-C45C	124.2(13)
N1C-Ru1C-P1C-C45C	102.73(13)
C1C-Ru1C-P1C-C51C	170.74(13)
N3C-Ru1C-P1C-C51C	73.98(13)
O1C-Ru1C-P1C-C51C	-109.52(12)
N5C-Ru1C-P1C-C51C	7.1(14)

N1C-Ru1C-P1C-C51C	-14.37(12)
C1C-Ru1C-O1C-C16C	4.4(2)
N3C-Ru1C-O1C-C16C	62.4(7)
N5C-Ru1C-O1C-C16C	93.3(2)
N1C-Ru1C-O1C-C16C	176.24(19)
P1C-Ru1C-O1C-C16C	-89.35(19)
C1C-Ru1C-N1C-C30C	96.4(7)
N3C-Ru1C-N1C-C30C	-144.9(3)
O1C-Ru1C-N1C-C30C	41.9(3)
N5C-Ru1C-N1C-C30C	128.7(3)
P1C-Ru1C-N1C-C30C	-52.4(3)
C1C-Ru1C-N1C-N2C	-80.2(6)
N3C-Ru1C-N1C-N2C	38.6(2)
O1C-Ru1C-N1C-N2C	-134.6(2)
N5C-Ru1C-N1C-N2C	-47.8(2)
P1C-Ru1C-N1C-N2C	131.07(19)
C30C-N1C-N2C-C32C	-0.4(3)
Ru1C-N1C-N2C-C32C	177.1(2)
C30C-N1C-N2C-B1C	-173.6(3)
Ru1C-N1C-N2C-B1C	3.9(3)
C1C-Ru1C-N3C-C33C	-45.2(3)
O1C-Ru1C-N3C-C33C	-102.3(7)
N5C-Ru1C-N3C-C33C	-133.2(3)
N1C-Ru1C-N3C-C33C	143.5(3)
P1C-Ru1C-N3C-C33C	49.5(3)
C1C-Ru1C-N3C-N4C	133.7(2)
O1C-Ru1C-N3C-N4C	76.6(7)
N5C-Ru1C-N3C-N4C	45.6(2)
N1C-Ru1C-N3C-N4C	-37.6(2)
P1C-Ru1C-N3C-N4C	-131.6(2)
C33C-N3C-N4C-C35C	-0.4(3)
Ru1C-N3C-N4C-C35C	-179.6(2)
C33C-N3C-N4C-B1C	174.3(3)
Ru1C-N3C-N4C-B1C	-4.8(3)
C1C-Ru1C-N5C-C36C	45.8(3)
N3C-Ru1C-N5C-C36C	142.4(3)
O1C-Ru1C-N5C-C36C	-33.8(3)
N1C-Ru1C-N5C-C36C	-129.0(3)
P1C-Ru1C-N5C-C36C	-150.5(12)
C1C-Ru1C-N5C-N6C	-139.2(2)
N3C-Ru1C-N5C-N6C	-42.6(2)
O1C-Ru1C-N5C-N6C	141.3(2)
N1C-Ru1C-N5C-N6C	46.1(2)
P1C-Ru1C-N5C-N6C	24.5(15)
C36C-N5C-N6C-C38C	0.4(3)
Ru1C-N5C-N6C-C38C	-175.9(2)
C36C-N5C-N6C-B1C	175.0(3)
Ru1C-N5C-N6C-B1C	-1.3(3)
C32C-N2C-B1C-N6C	-113.8(4)
N1C-N2C-B1C-N6C	57.9(3)
C32C-N2C-B1C-N4C	128.4(3)
N1C-N2C-B1C-N4C	-59.9(4)
C38C-N6C-B1C-N2C	112.8(3)
N5C-N6C-B1C-N2C	-60.4(3)
C38C-N6C-B1C-N4C	-129.5(3)
N5C-N6C-B1C-N4C	57.4(3)
C35C-N4C-B1C-N2C	-124.2(3)
N3C-N4C-B1C-N2C	62.3(4)
C35C-N4C-B1C-N6C	118.9(3)
N3C-N4C-B1C-N6C	-54.6(3)
C16C-O2C-C1C-C2C	-161.1(3)
C16C-O2C-C1C-Ru1C	13.0(3)
N3C-Ru1C-C1C-C2C	-11.2(4)
O1C-Ru1C-C1C-C2C	162.5(4)
N5C-Ru1C-C1C-C2C	74.8(4)
N1C-Ru1C-C1C-C2C	107.0(6)
P1C-Ru1C-C1C-C2C	-104.3(4)
N3C-Ru1C-C1C-O2C	177.60(17)
O1C-Ru1C-C1C-O2C	-8.72(16)
N5C-Ru1C-C1C-O2C	-96.37(18)
N1C-Ru1C-C1C-O2C	-64.3(7)
P1C-Ru1C-C1C-O2C	84.46(17)
O2C-C1C-C2C-C3C	-3.7(4)
Ru1C-C1C-C2C-C3C	-174.9(2)
C1C-C2C-C3C-C10C	-125.3(3)
C1C-C2C-C3C-C4C	109.8(4)
C2C-C3C-C4C-C5C	-16.3(4)
C10C-C3C-C4C-C5C	-141.4(3)
C2C-C3C-C4C-C9C	166.8(4)
C10C-C3C-C4C-C9C	41.7(5)
C9C-C4C-C5C-C6C	-3.0(6)
C3C-C4C-C5C-C6C	-179.9(3)
C4C-C5C-C6C-C7C	1.8(6)
C5C-C6C-C7C-C8C	0.8(7)
C6C-C7C-C8C-C9C	-2.2(10)
C7C-C8C-C9C-C4C	1.0(10)
C5C-C4C-C9C-C8C	1.6(8)
C3C-C4C-C9C-C8C	178.6(5)
C2C-C3C-C10C-C15C	120.3(3)
C4C-C3C-C10C-C15C	-112.7(3)
C2C-C3C-C10C-C11C	-61.8(4)
C4C-C3C-C10C-C11C	65.2(4)
C15C-C10C-C11C-C12C	1.4(5)
C3C-C10C-C11C-C12C	-176.6(3)
C10C-C11C-C12C-C13C	-0.4(5)
C11C-C12C-C13C-C14C	-1.0(5)
C12C-C13C-C14C-C15C	1.4(5)
C13C-C14C-C15C-C10C	-0.4(5)
C11C-C10C-C15C-C14C	-0.9(5)
C3C-C10C-C15C-C14C	177.0(3)
Ru1C-O1C-C16C-O2C	2.4(3)
Ru1C-O1C-C16C-C17C	-169.6(2)
C1C-O2C-C16C-O1C	-10.4(4)
C1C-O2C-C16C-C17C	162.0(2)
O1C-C16C-C17C-C24C	-137.0(3)
O2C-C16C-C17C-C24C	50.5(4)
O1C-C16C-C17C-C18C	97.1(3)
O2C-C16C-C17C-C18C	-75.4(3)

C16C-C17C-C18C-C19C	-99.7(3)
C24C-C17C-C18C-C19C	133.5(3)
C16C-C17C-C18C-C23C	75.0(3)
C24C-C17C-C18C-C23C	-51.8(4)
C23C-C18C-C19C-C20C	-1.2(5)
C17C-C18C-C19C-C20C	173.6(3)
C18C-C19C-C20C-C21C	-0.9(5)
C19C-C20C-C21C-C22C	2.0(6)
C20C-C21C-C22C-C23C	-1.0(6)
C21C-C22C-C23C-C18C	-1.1(5)
C19C-C18C-C23C-C22C	2.2(5)
C17C-C18C-C23C-C22C	-172.6(3)
C16C-C17C-C24C-C25C	-161.7(3)
C18C-C17C-C24C-C25C	-41.1(4)
C16C-C17C-C24C-C29C	20.7(4)
C18C-C17C-C24C-C29C	141.3(3)
C29C-C24C-C25C-C26C	-1.7(5)
C17C-C24C-C25C-C26C	-179.4(3)
C24C-C25C-C26C-C27C	0.5(5)
C25C-C26C-C27C-C28C	0.9(5)
C26C-C27C-C28C-C29C	-1.0(5)
C27C-C28C-C29C-C24C	-0.2(5)
C25C-C24C-C29C-C28C	1.5(5)
C17C-C24C-C29C-C28C	179.1(3)
N2C-N1C-C30C-C31C	0.7(3)
Ru1C-N1C-C30C-C31C	-176.1(2)
N1C-C30C-C31C-C32C	-0.7(4)
N1C-N2C-C32C-C31C	-0.1(4)
B1C-N2C-C32C-C31C	172.2(3)
C30C-C31C-C32C-N2C	0.5(4)
N4C-N3C-C33C-C34C	0.7(3)
Ru1C-N3C-C33C-C34C	179.7(2)
N3C-C33C-C34C-C35C	-0.7(4)
N3C-N4C-C35C-C34C	0.0(4)
B1C-N4C-C35C-C34C	-174.1(3)
C33C-C34C-C35C-N4C	0.4(4)
N6C-N5C-C36C-C37C	-0.5(4)
Ru1C-N5C-C36C-C37C	175.0(2)
N5C-C36C-C37C-C38C	0.4(4)
N5C-N6C-C38C-C37C	-0.2(4)
B1C-N6C-C38C-C37C	-174.0(3)
C36C-C37C-C38C-N6C	-0.1(4)
C45C-P1C-C39C-C40C	-101.4(3)
C51C-P1C-C39C-C40C	3.1(3)
Ru1C-P1C-C39C-C40C	128.6(2)
C45C-P1C-C39C-C44C	77.2(3)
C51C-P1C-C39C-C44C	-178.2(2)
Ru1C-P1C-C39C-C44C	-52.7(3)
C44C-C39C-C40C-C41C	-1.1(5)
P1C-C39C-C40C-C41C	177.6(2)
C39C-C40C-C41C-C42C	0.8(5)
C40C-C41C-C42C-C43C	0.4(5)
C41C-C42C-C43C-C44C	-1.2(5)
C42C-C43C-C44C-C39C	0.9(5)
C40C-C39C-C44C-C43C	0.3(4)
P1C-C39C-C44C-C43C	-178.5(2)
C39C-P1C-C45C-C46C	0.9(3)
C51C-P1C-C45C-C46C	-104.7(3)
Ru1C-P1C-C45C-C46C	132.6(2)
C39C-P1C-C45C-C50C	178.2(2)
C51C-P1C-C45C-C50C	72.7(3)
Ru1C-P1C-C45C-C50C	-50.1(3)
C50C-C45C-C46C-C47C	2.1(5)
P1C-C45C-C46C-C47C	179.5(3)
C45C-C46C-C47C-C48C	-2.1(5)
C46C-C47C-C48C-C49C	0.3(5)
C47C-C48C-C49C-C50C	1.5(5)
C48C-C49C-C50C-C45C	-1.5(5)
C46C-C45C-C50C-C49C	-0.2(4)
P1C-C45C-C50C-C49C	-177.8(2)
C39C-P1C-C51C-C52C	-105.0(3)
C45C-P1C-C51C-C52C	-1.4(3)
Ru1C-P1C-C51C-C52C	124.7(2)
C39C-P1C-C51C-C56C	80.8(3)
C45C-P1C-C51C-C56C	-175.6(2)
Ru1C-P1C-C51C-C56C	-49.5(3)
C56C-C51C-C52C-C53C	1.7(4)
P1C-C51C-C52C-C53C	-172.6(2)
C51C-C52C-C53C-C54C	-1.2(5)
C52C-C53C-C54C-C55C	0.2(5)
C53C-C54C-C55C-C56C	0.2(5)
C54C-C55C-C56C-C51C	0.4(5)
C52C-C51C-C56C-C55C	-1.3(5)
P1C-C51C-C56C-C55C	173.2(2)
C6-C1-C2-C3	0.0
C7#1-C1-C2-C3	0.3(9)
C1-C2-C3-C4	0.0
C2-C3-C4-C5	0.0
C3-C4-C5-C6	0.0
C4-C5-C6-C1	0.0
C4-C5-C6-C7	180.0
C2-C1-C6-C5	0.0
C7#1-C1-C6-C5	-0.1(4)
C2-C1-C6-C7	180.0
C7#1-C1-C6-C7	179.9(4)
C5-C6-C7-C1#1	0.2(8)
C1-C6-C7-C1#1	-179.8(8)
C9-C10-C11-C12	-174.1(4)
C10-C11-C12-C13	-65.5(6)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+2,-z+1

Table 13. Crystal data and structure refinement for 7 CCDC 165163 MSS22.

Empirical formula	$C_{34}H_{30}BCl_3N_6PRu$ (CH_2Cl_2, C_7H_8)
Formula weight	817.89
Crystallization Solvent	Dichloromethane/pentane
Crystal Habit	Feathered blocks
Crystal size	0.33 x 0.26 x 0.19 mm^3
Crystal color	Emerald green

Data Collection

Type of diffractometer	CCD area detector
Wavelength	0.71073 Å MoKα
Data Collection Temperature	98(2) K
θ range for 5706 reflections used in lattice determination	2.17 to 23.26°
Unit cell dimensions	a = 10.0980(6) Å b = 30.0953(17) Å β= 90.2250(10)° c = 11.9758(7) Å
Volume	3639.4(4) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/n$
Density (calculated)	1.493 Mg/m^3
F(000)	1658
θ range for data collection	1.83 to 23.27°
Completeness to θ = 23.27°	99.8 %
Index ranges	$-11 \le h \le 11$, $-33 \le k \le 33$, $-13 \le l \le 13$
Data collection scan type	ω scans at 3 ϕ settings
Reflections collected	25421
Independent reflections	5225 [R_{int}= 0.0504]
Absorption coefficient	0.732 mm^{-1}
Absorption correction	None

Table 13 (cont.)

Structure solution and Refinement

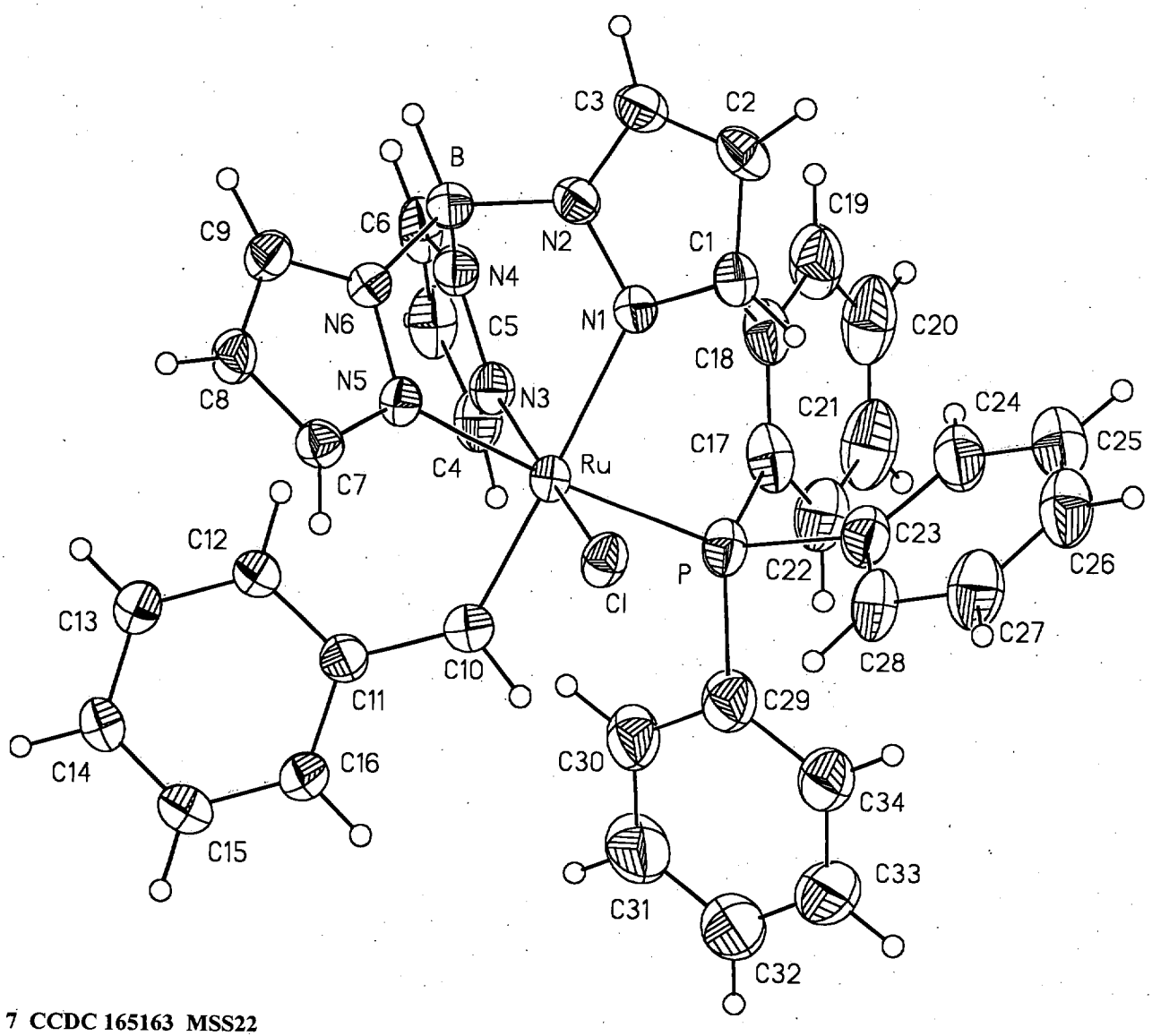
Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Calculated geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	5225 / 6 / 418
Treatment of hydrogen atoms	Restrained
Goodness-of-fit on F^2	1.027
Final R indices [$I>2\sigma(I)$]	R1 = 0.0670, *w*R2 = 0.1784
R indices (all data)	R1 = 0.0708, *w*R2 = 0.1815
Type of weighting scheme used	Calculated weights
Weighting scheme used	$w=1/[\sigma^2(Fo^2)+(0.0924P)^2+28.8470P]$ where $P=(Fo^2+2Fc^2)/3$
Max shift/error	0.209
Average shift/error	0.006
Largest diff. peak and hole	2.610 and -1.157 e.Å^{-3}

Special Refinement Details

The crystal lattice contains a poorly defined region of included solvent. This region was modeled with dichloromethane or toluene at this site. This model of the ruthenium moiety contains no difference peaks greater than one electron but the model of the solvent region contains large difference peaks but the region is so confused as to make it impossible to resolve.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.



7 CCDC 165163 MSS22

Table 14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 7 CCDC 165163 MSS22. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Ru	9489(2)	8283(1)	7773(1)	24(1)	1
Cl	11849(5)	8188(2)	7598(4)	32(1)	1
P	9662(6)	8992(2)	8553(5)	32(1)	1
N(1)	9652(16)	7962(5)	9404(13)	26(4)	1
N(2)	8750(16)	7639(6)	9676(13)	30(4)	1
N(3)	7447(17)	8267(5)	7974(14)	30(4)	1
N(4)	6879(16)	7904(6)	8462(14)	31(4)	1
N(5)	9318(15)	7622(5)	7217(13)	26(4)	1
N(6)	8466(16)	7343(5)	7737(13)	27(4)	1
B	7720(20)	7498(8)	8792(19)	31(5)	1
C(1)	10500(20)	7985(7)	10261(17)	30(5)	1
C(2)	10140(20)	7685(8)	11088(18)	38(5)	1
C(3)	9040(20)	7474(8)	10687(17)	37(5)	1
C(4)	6460(20)	8541(8)	7706(19)	38(5)	1
C(5)	5240(20)	8359(8)	8020(20)	42(6)	1
C(6)	5550(20)	7962(8)	8486(18)	37(5)	1
C(7)	9860(20)	7396(7)	6383(17)	30(5)	1
C(8)	9360(20)	6968(7)	6347(17)	33(5)	1
C(9)	8480(20)	6944(7)	7218(18)	33(5)	1
C(10)	9510(20)	8510(7)	6294(17)	33(5)	1
C(11)	8870(20)	8371(7)	5257(18)	32(5)	1
C(12)	7780(20)	8078(7)	5203(17)	35(5)	1
C(13)	7270(20)	7939(8)	4188(19)	42(6)	1
C(14)	7840(30)	8085(8)	3203(19)	48(6)	1
C(15)	8890(30)	8377(8)	3220(20)	48(6)	1
C(16)	9410(20)	8516(7)	4234(18)	39(5)	1
C(17)	8260(20)	9152(8)	9453(19)	44(6)	1
C(18)	7780(20)	8841(8)	10218(19)	43(6)	1
C(19)	6860(30)	8968(10)	11010(20)	55(7)	1
C(20)	6400(30)	9411(10)	11020(30)	63(8)	1
C(21)	6840(30)	9715(10)	10240(30)	64(8)	1
C(22)	7790(20)	9590(8)	9460(20)	49(6)	1
C(23)	11030(20)	9077(7)	9560(19)	41(6)	1
C(24)	10790(30)	9161(8)	10690(20)	48(6)	1
C(25)	11840(30)	9187(9)	11450(20)	53(7)	1
C(26)	13120(30)	9133(9)	11070(20)	55(7)	1
C(27)	13370(30)	9065(9)	9940(20)	55(7)	1
C(28)	12320(20)	9041(8)	9180(20)	43(6)	1
C(29)	9780(30)	9472(8)	7640(20)	47(6)	1
C(30)	8830(30)	9508(8)	6770(20)	52(7)	1
C(31)	8820(40)	9883(9)	6110(20)	70(9)	1
C(32)	9740(40)	10220(9)	6260(20)	68(9)	1
C(33)	10690(30)	10185(9)	7110(20)	61(8)	1
C(34)	10690(30)	9817(8)	7800(20)	50(6)	1
C(100)	4660(30)	8724(8)	4340(110)	115(10)	0.39(3)
Cl(10)	3120(20)	8991(11)	4440(30)	115(10)	0.39(3)
Cl(11)	5970(20)	9104(11)	4290(30)	115(10)	0.39(3)
C(200)	5126(1)	9783(5)	7101(16)	210(20)	0.61(3)

C(201)	4530(50)	9431(9)	6300(20)	210(20)	0.61(3)
C(202)	5340(70)	9170(20)	5630(50)	210(20)	0.61(3)
C(203)	4790(90)	8860(20)	4920(50)	210(20)	0.61(3)
C(204)	3420(100)	8803(19)	4870(50)	210(20)	0.61(3)
C(205)	2610(70)	9060(30)	5530(60)	210(20)	0.61(3)
C(206)	3160(60)	9380(20)	6250(50)	210(20)	0.61(3)

Table 15. Selected bond lengths [Å] and angles [°] for 7 CCDC 165163 MSS22.

Ru-C(10)	1.90(2)	N(3)-Ru-N(1)	87.5(6)
Ru-N(3)	2.077(17)	N(5)-Ru-N(1)	82.5(6)
Ru-N(5)	2.105(16)	C(10)-Ru-P	92.5(7)
Ru-N(1)	2.186(16)	N(3)-Ru-P	92.7(5)
Ru-P	2.335(6)	N(5)-Ru-P	174.8(5)
Ru-Cl	2.410(5)	N(1)-Ru-P	92.3(4)
		C(10)-Ru-Cl	87.0(7)
C(10)-Ru-N(3)	97.5(8)	N(3)-Ru-Cl	171.7(5)
C(10)-Ru-N(5)	92.7(8)	N(5)-Ru-Cl	86.6(4)
N(3)-Ru-N(5)	86.2(6)	N(1)-Ru-Cl	87.4(4)
C(10)-Ru-N(1)	172.9(8)	P-Ru-Cl	94.05(19)

Table 16. Bond lengths [Å] and angles [°] for 7 CCDC 165163 MSS22.

Ru-C(10)	1.90(2)	C(100)-C(205)	2.72(11)
Ru-N(3)	2.077(17)	C(100)-C(203)	0.80(12)
Ru-N(5)	2.105(16)	C(100)-Cl(11)	1.750(3)
Ru-N(1)	2.186(16)	C(100)-Cl(10)	1.750(3)
Ru-P	2.335(6)	Cl(10)-C(205)	1.43(9)
Ru-Cl	2.410(5)	Cl(10)-C(204)	0.82(8)
P-C(29)	1.82(3)	Cl(10)-C(206)	2.46(6)
P-C(23)	1.85(2)	Cl(11)-C(203)	1.60(10)
P-C(17)	1.85(2)	Cl(11)-C(204)	2.81(10)
N(1)-C(1)	1.33(3)	Cl(11)-C(202)	1.74(6)
N(1)-N(2)	1.37(2)	C(200)-C(201)	1.5515
N(2)-C(3)	1.34(3)	C(201)-C(202)	1.3900
N(2)-B	1.54(3)	C(201)-C(206)	1.3900
N(3)-C(4)	1.33(3)	C(202)-C(203)	1.3900
N(3)-N(4)	1.37(2)	C(203)-C(204)	1.3900
N(4)-C(6)	1.35(3)	C(204)-C(205)	1.3900
N(4)-B	1.54(3)	C(205)-C(206)	1.3900
N(5)-C(7)	1.33(3)		
N(5)-N(6)	1.36(2)	C(10)-Ru-N(3)	97.5(8)
N(6)-C(9)	1.35(3)	C(10)-Ru-N(5)	92.7(8)
N(6)-B	1.55(3)	N(3)-Ru-N(5)	86.2(6)
C(1)-C(2)	1.39(3)	C(10)-Ru-N(1)	172.9(8)
C(2)-C(3)	1.36(3)	N(3)-Ru-N(1)	87.5(6)
C(4)-C(5)	1.40(3)	N(5)-Ru-N(1)	82.5(6)
C(5)-C(6)	1.35(4)	C(10)-Ru-P	92.5(7)
C(7)-C(8)	1.39(3)	N(3)-Ru-P	92.7(5)
C(8)-C(9)	1.38(3)	N(5)-Ru-P	174.8(5)
C(10)-C(11)	1.46(3)	N(1)-Ru-P	92.3(4)
C(11)-C(16)	1.41(3)	C(10)-Ru-Cl	87.0(7)
C(11)-C(12)	1.41(3)	N(3)-Ru-Cl	171.7(5)
C(12)-C(13)	1.38(3)	N(5)-Ru-Cl	86.6(4)
C(13)-C(14)	1.39(3)	N(1)-Ru-Cl	87.4(4)
C(14)-C(15)	1.38(4)	P-Ru-Cl	94.05(19)
C(15)-C(16)	1.38(3)	C(29)-P-C(23)	103.6(11)
C(17)-C(18)	1.40(4)	C(29)-P-C(17)	101.2(12)
C(17)-C(22)	1.40(3)	C(23)-P-C(17)	99.0(11)
C(18)-C(19)	1.38(3)	C(29)-P-Ru	119.3(8)
C(19)-C(20)	1.41(4)	C(23)-P-Ru	116.2(7)
C(20)-C(21)	1.38(5)	C(17)-P-Ru	114.5(8)
C(21)-C(22)	1.39(4)	C(1)-N(1)-N(2)	106.2(16)
C(23)-C(28)	1.39(3)	C(1)-N(1)-Ru	135.3(14)
C(23)-C(24)	1.40(3)	N(2)-N(1)-Ru	118.5(12)
C(24)-C(25)	1.39(4)	C(3)-N(2)-N(1)	109.3(17)
C(25)-C(26)	1.37(4)	C(3)-N(2)-B	131.6(18)
C(26)-C(27)	1.39(4)	N(1)-N(2)-B	118.7(16)
C(27)-C(28)	1.40(3)	C(4)-N(3)-N(4)	106.5(17)
C(29)-C(34)	1.40(4)	C(4)-N(3)-Ru	134.3(15)
C(29)-C(30)	1.41(4)	N(4)-N(3)-Ru	119.2(12)
C(30)-C(31)	1.38(4)	C(6)-N(4)-N(3)	108.9(18)
C(31)-C(32)	1.39(4)	C(6)-N(4)-B	130.0(19)
C(32)-C(33)	1.39(4)	N(3)-N(4)-B	120.9(16)
C(33)-C(34)	1.38(4)	C(7)-N(5)-N(6)	107.0(16)

C(7)-N(5)-Ru	133.5(14)	C(34)-C(33)-C(32)	120(3)
N(6)-N(5)-Ru	119.5(12)	C(33)-C(34)-C(29)	121(3)
C(9)-N(6)-N(5)	109.5(16)	C(205)-C(100)-C(203)	59(7)
C(9)-N(6)-B	130.4(17)	C(205)-C(100)-Cl(11)	111(3)
N(5)-N(6)-B	120.0(16)	C(203)-C(100)-Cl(11)	66(7)
N(4)-B-N(2)	109.1(17)	C(205)-C(100)-Cl(10)	28(3)
N(4)-B-N(6)	107.5(17)	C(203)-C(100)-Cl(10)	82(7)
N(2)-B-N(6)	108.3(17)	Cl(11)-C(100)-Cl(10)	111.9(3)
N(1)-C(1)-C(2)	110.5(19)	C(205)-Cl(10)-C(204)	70(6)
C(3)-C(2)-C(1)	105.2(19)	C(205)-Cl(10)-C(100)	117(5)
N(2)-C(3)-C(2)	108.8(19)	C(204)-Cl(10)-C(100)	53(8)
N(3)-C(4)-C(5)	110(2)	C(205)-Cl(10)-C(206)	28.7(9)
C(6)-C(5)-C(4)	105(2)	C(204)-Cl(10)-C(206)	76(4)
C(5)-C(6)-N(4)	109(2)	C(100)-Cl(10)-C(206)	105(4)
N(5)-C(7)-C(8)	110.4(18)	C(203)-Cl(11)-C(204)	18(2)
C(9)-C(8)-C(7)	105.1(18)	C(203)-Cl(11)-C(100)	27(4)
N(6)-C(9)-C(8)	108.0(18)	C(204)-Cl(11)-C(100)	24(2)
C(11)-C(10)-Ru	133.2(16)	C(203)-Cl(11)-C(202)	49(2)
C(16)-C(11)-C(12)	117.0(19)	C(204)-Cl(11)-C(202)	58(3)
C(16)-C(11)-C(10)	119(2)	C(100)-Cl(11)-C(202)	76(4)
C(12)-C(11)-C(10)	124.1(19)	C(202)-C(201)-C(206)	120.0
C(13)-C(12)-C(11)	121(2)	C(202)-C(201)-C(200)	121(3)
C(12)-C(13)-C(14)	120(2)	C(206)-C(201)-C(200)	119(3)
C(15)-C(14)-C(13)	121(2)	C(201)-C(202)-C(203)	120.00(11)
C(14)-C(15)-C(16)	120(2)	C(201)-C(202)-Cl(11)	144(5)
C(15)-C(16)-C(11)	122(2)	C(203)-C(202)-Cl(11)	60(3)
C(18)-C(17)-C(22)	120(2)	Cl(11)-C(203)-C(204)	141(5)
C(18)-C(17)-P	118.6(18)	Cl(11)-C(203)-C(202)	71(3)
C(22)-C(17)-P	121(2)	C(204)-C(203)-C(202)	120.0
C(19)-C(18)-C(17)	120(2)	Cl(11)-C(203)-C(100)	87(8)
C(18)-C(19)-C(20)	119(3)	C(204)-C(203)-C(100)	75(8)
C(21)-C(20)-C(19)	121(3)	C(202)-C(203)-C(100)	158(9)
C(20)-C(21)-C(22)	120(3)	C(203)-C(204)-C(205)	120.0
C(21)-C(22)-C(17)	120(3)	C(203)-C(204)-Cl(10)	108(7)
C(28)-C(23)-C(24)	120(2)	C(205)-C(204)-Cl(10)	76(7)
C(28)-C(23)-P	118.3(18)	C(203)-C(204)-Cl(11)	21(3)
C(24)-C(23)-P	122(2)	C(205)-C(204)-Cl(11)	120.2(18)
C(23)-C(24)-C(25)	120(3)	Cl(10)-C(204)-Cl(11)	88(6)
C(26)-C(25)-C(24)	119(3)	Cl(10)-C(205)-C(206)	122(3)
C(25)-C(26)-C(27)	121(2)	Cl(10)-C(205)-C(204)	34(4)
C(26)-C(27)-C(28)	120(3)	C(206)-C(205)-C(204)	120.00(10)
C(23)-C(28)-C(27)	119(2)	Cl(10)-C(205)-C(100)	35(3)
C(34)-C(29)-C(30)	119(2)	C(206)-C(205)-C(100)	106(2)
C(34)-C(29)-P	123.4(19)	C(204)-C(205)-C(100)	14.8(18)
C(30)-C(29)-P	117.4(19)	C(205)-C(206)-C(201)	120.00(7)
C(31)-C(30)-C(29)	119(3)	C(205)-C(206)-Cl(10)	30(2)
C(30)-C(31)-C(32)	121(3)	C(201)-C(206)-Cl(10)	96(3)
C(33)-C(32)-C(31)	120(3)		

Table 17. Anisotropic displacement parameters ($Å^2 x 10^4$) for 7 CCDC 165163 MSS22. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru	240(10)	235(10)	246(10)	-24(6)	-13(7)	-2(6)
Cl	250(30)	320(30)	370(30)	-80(20)	30(20)	-20(20)
P	350(30)	280(30)	340(30)	-50(20)	-70(20)	30(20)
N(1)	270(90)	260(90)	260(90)	-10(70)	-20(70)	10(70)
N(2)	300(90)	340(100)	250(90)	0(70)	20(70)	-20(80)
N(3)	280(90)	300(100)	300(90)	-50(70)	-10(80)	20(70)
N(4)	270(90)	380(100)	280(90)	-50(80)	30(70)	-50(80)
N(5)	240(90)	270(90)	270(90)	-40(70)	-10(70)	0(70)
N(6)	280(90)	270(90)	260(90)	10(70)	0(70)	-40(70)
B	300(120)	350(130)	270(120)	-10(100)	30(100)	-70(100)
C(1)	300(110)	310(110)	290(110)	-50(90)	-20(90)	20(90)
C(2)	390(130)	490(140)	250(110)	40(100)	-50(90)	40(100)
C(3)	430(130)	380(120)	290(110)	30(100)	40(100)	-10(100)
C(4)	340(120)	380(130)	410(130)	-90(100)	-80(100)	60(100)
C(5)	260(120)	540(150)	460(140)	-190(120)	-40(100)	80(100)
C(6)	200(110)	570(150)	340(120)	-180(110)	10(90)	-20(100)
C(7)	270(110)	340(120)	280(110)	-10(90)	20(90)	0(90)
C(8)	400(120)	260(110)	330(110)	-80(90)	0(90)	10(90)
C(9)	380(120)	270(110)	350(120)	0(90)	-40(90)	-50(90)
C(10)	350(120)	310(110)	310(110)	20(90)	0(90)	-40(90)
C(11)	420(120)	250(100)	300(110)	10(90)	-20(90)	10(90)
C(12)	440(130)	330(120)	260(110)	40(90)	-40(90)	-70(100)
C(13)	520(140)	370(130)	370(130)	10(100)	-80(110)	-140(110)
C(14)	660(170)	490(150)	270(120)	-10(110)	-90(110)	-180(130)
C(15)	680(170)	460(140)	290(120)	50(110)	-10(120)	-130(130)
C(16)	520(140)	300(120)	350(120)	30(90)	-40(100)	-100(100)
C(17)	480(140)	450(140)	380(130)	-130(110)	-90(110)	70(110)
C(18)	530(150)	410(130)	360(130)	-130(110)	-60(110)	40(110)
C(19)	520(160)	620(180)	500(150)	-250(130)	90(120)	-40(130)
C(20)	450(150)	700(200)	700(200)	-390(170)	20(140)	20(140)
C(21)	560(170)	530(170)	800(200)	-340(160)	-70(160)	100(140)
C(22)	470(140)	410(140)	590(160)	-120(120)	-80(120)	40(110)
C(23)	500(140)	310(120)	420(130)	-30(100)	-120(110)	0(100)
C(24)	590(160)	450(140)	410(140)	-60(110)	-120(120)	0(120)
C(25)	620(170)	480(150)	480(150)	-90(120)	-130(130)	100(130)
C(26)	640(180)	440(150)	570(170)	-100(120)	-230(140)	100(130)
C(27)	540(160)	460(150)	670(180)	-160(130)	-130(130)	100(120)
C(28)	400(130)	380(130)	500(140)	-170(110)	-90(110)	50(100)
C(29)	610(160)	350(130)	450(140)	-50(110)	-40(120)	20(110)
C(30)	790(190)	330(130)	450(140)	-20(110)	-170(130)	20(120)
C(31)	1200(300)	430(160)	510(160)	90(130)	-220(170)	30(170)
C(32)	1200(300)	310(140)	510(170)	30(120)	-70(170)	0(160)
C(33)	900(200)	350(140)	600(180)	-30(120)	60(160)	-40(140)
C(34)	670(170)	360(130)	470(150)	-70(110)	-10(130)	-10(120)

Table 18. Torsion angles [°] for 7 CCDC 165163 MSS22.

P-Ru-C(1)-H(1)	-50.5

Table 19. Crystal data and structure refinement for 8 CCDC 133554 MSS15.

Empirical formula	$C_{49}H_{41}BN_6O_2PRu$ (C_7H_8)
Formula weight	980.86
Crystallization Solvent	Toluene
Crystal Habit	Lozenge
Crystal size	0.15 x 0.29 x 0.37 mm^3
Crystal color	Yellow/Orange

Data Collection

Preliminary Photos	Rotation
Type of diffractometer	CCD area detector
Wavelength	0.71073 Å MoKα
Data Collection Temperature	293(2) K
θ range for reflections used in lattice determination	2.3 to 28.1° (7633 reflections)
Unit cell dimensions	a = 13.7367(7) Å α= 90° b = 19.5683(10) Å β= 102.091(1)° c = 18.5679(10) Å γ = 90°
Volume	4880.4(4) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/n$
Density (calculated)	1.335 Mg/m^3
F(000)	2028
θ range for data collection	1.53 to 28.53°
Completeness to θ = 28.53°	92.2 %
Index ranges	$-17 \le h \le 17, -26 \le k \le 26, -24 \le l \le 24$
Data collection scan type	φ and ω scans
Reflections collected	47152
Independent reflections	11439 [R_{int}= 0.0418]
Absorption coefficient	0.403 mm^{-1}
Absorption correction	None
Variation of standards	Within counting stastistcs, zero%.

Table 19 (cont.)

Structure solution and Refinement

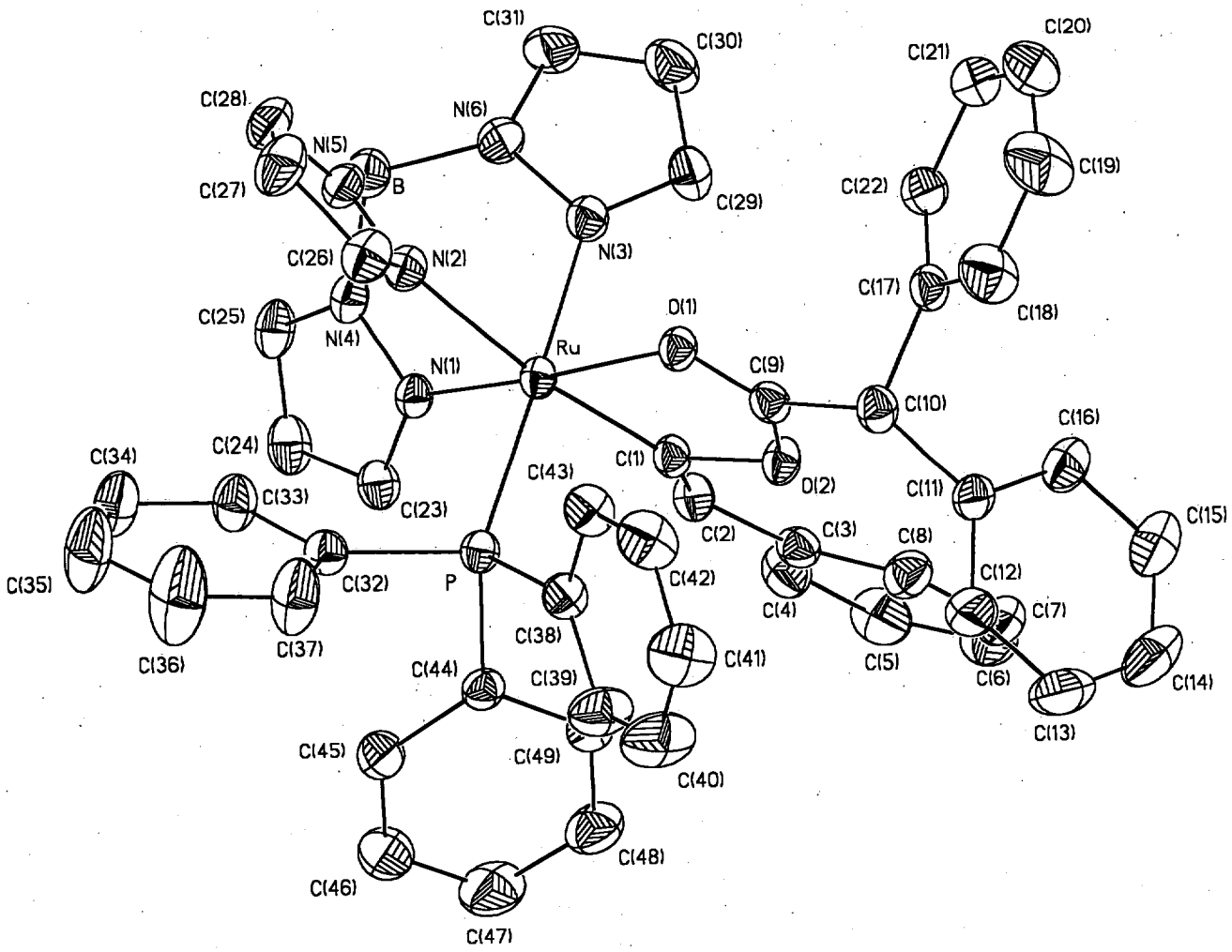
Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Calculated geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	11439 / 5 / 556
Treatment of hydrogen atoms	Restrained
Goodness-of-fit on F^2	2.642
Final R indices [$I>2\sigma(I)$]	R1 = 0.0420, wR2 = 0.0853
R indices (all data)	R1 = 0.0586, wR2 = 0.0866
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	2.417
Average shift/error	0.045
Largest diff. peak and hole	0.765 and -0.842 e.Å^{-3}

Special Refinement Details

The crystal contains one site in the asymmetric unit occupied by a disordered toluene. There are two orientations of the toluene and the sum of their occupancies was constrained to total one. Each orientation was refined as a rigid body with one overall temperature factor.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.



8 CCDC 133554 MSS15

Table 20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 8 CCDC 133554 MSS15. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Ru	1539(1)	7665(1)	69(1)	40(1)	1
P	3151(1)	8055(1)	329(1)	43(1)	1
O(1)	1946(1)	6729(1)	-345(1)	45(1)	1
O(2)	2162(1)	6411(1)	836(1)	48(1)	1
N(1)	1009(2)	8514(1)	503(1)	43(1)	1
N(2)	1161(2)	8186(1)	-998(1)	50(1)	1
N(3)	32(2)	7335(1)	-157(1)	48(1)	1
N(4)	151(2)	8810(1)	120(1)	50(1)	1
N(5)	268(2)	8522(1)	-1165(1)	53(1)	1
N(6)	-694(2)	7776(1)	-479(1)	57(1)	1
B	-430(3)	8521(2)	-621(2)	58(1)	1
C(1)	1735(2)	7096(1)	969(1)	42(1)	1
C(2)	1515(2)	7136(1)	1633(1)	49(1)	1
C(3)	1607(2)	6678(1)	2269(1)	48(1)	1
C(4)	1202(2)	6899(2)	2855(2)	65(1)	1
C(5)	1245(3)	6500(2)	3478(2)	80(1)	1
C(6)	1696(3)	5875(2)	3528(2)	81(1)	1
C(7)	2110(2)	5657(2)	2964(2)	75(1)	1
C(8)	2072(2)	6048(2)	2338(2)	59(1)	1
C(9)	2217(2)	6307(1)	149(2)	44(1)	1
C(10)	2692(2)	5632(1)	-6(2)	50(1)	1
C(11)	3158(2)	5231(1)	673(2)	52(1)	1
C(12)	4152(3)	5309(2)	978(2)	80(1)	1
C(13)	4598(3)	4924(2)	1584(2)	100(1)	1
C(14)	4043(4)	4471(2)	1877(2)	101(2)	1
C(15)	3059(3)	4393(2)	1595(2)	86(1)	1
C(16)	2624(3)	4773(2)	991(2)	68(1)	1
C(17)	1998(2)	5195(1)	-574(1)	48(1)	1
C(18)	2415(3)	4739(2)	-985(2)	85(1)	1
C(19)	1821(4)	4321(2)	-1496(2)	105(1)	1
C(20)	812(4)	4353(2)	-1591(2)	90(1)	1
C(21)	394(3)	4785(2)	-1181(2)	76(1)	1
C(22)	989(2)	5208(2)	-677(2)	61(1)	1
C(23)	1286(2)	8875(1)	1120(2)	51(1)	1
C(24)	622(3)	9411(1)	1137(2)	62(1)	1
C(25)	-75(2)	9350(2)	513(2)	60(1)	1
C(26)	1576(2)	8267(2)	-1575(2)	62(1)	1
C(27)	963(3)	8644(2)	-2118(2)	78(1)	1
C(28)	144(3)	8789(2)	-1841(2)	66(1)	1
C(29)	-423(2)	6765(2)	-23(2)	61(1)	1
C(30)	-1444(2)	6827(2)	-257(2)	78(1)	1
C(31)	-1577(2)	7473(2)	-534(2)	75(1)	1
C(32)	3375(2)	8840(1)	-151(1)	48(1)	1
C(33)	2694(2)	9365(2)	-227(2)	63(1)	1
C(34)	2843(3)	9977(2)	-571(2)	81(1)	1
C(35)	3649(3)	10057(2)	-868(3)	115(2)	1
C(36)	4313(4)	9533(2)	-817(3)	147(2)	1

C(37)	4174(3)	8933(2)	-466(2)	98(1)	1
C(38)	4104(2)	7482(1)	97(2)	51(1)	1
C(39)	5020(2)	7374(2)	552(2)	81(1)	1
C(40)	5731(3)	6967(2)	315(2)	105(1)	1
C(41)	5531(3)	6664(2)	-348(2)	97(1)	1
C(42)	4624(3)	6763(2)	-804(2)	80(1)	1
C(43)	3915(2)	7170(1)	-587(2)	59(1)	1
C(44)	3693(2)	8270(1)	1292(1)	47(1)	1
C(45)	3997(2)	8927(2)	1518(2)	67(1)	1
C(46)	4339(3)	9079(2)	2256(2)	94(1)	1
C(47)	4406(3)	8580(2)	2772(2)	97(1)	1
C(48)	4140(3)	7925(2)	2565(2)	82(1)	1
C(49)	3777(2)	7769(2)	1824(2)	61(1)	1
C(51)	3236(3)	6787(2)	6876(2)	152(2)	0.728(5)
C(52)	2437(3)	7107(2)	7087(2)	152(2)	0.728(5)
C(53)	1845(3)	6745(3)	7477(3)	152(2)	0.728(5)
C(54)	2053(3)	6063(3)	7655(2)	152(2)	0.728(5)
C(55)	2852(4)	5743(2)	7443(3)	152(2)	0.728(5)
C(56)	3444(3)	6105(2)	7054(3)	152(2)	0.728(5)
C(50)	3878(4)	7226(3)	6468(3)	152(2)	0.728(5)
C(61)	2400(6)	6861(4)	7423(4)	125(3)	0.272(5)
C(62)	2676(8)	7467(4)	7131(6)	125(3)	0.272(5)
C(63)	3404(9)	7463(5)	6711(6)	125(3)	0.272(5)
C(64)	3856(8)	6852(6)	6584(6)	125(3)	0.272(5)
C(65)	3580(9)	6245(5)	6876(7)	125(3)	0.272(5)
C(66)	2852(8)	6250(4)	7295(6)	125(3)	0.272(5)
C(60)	1772(8)	6881(7)	8018(6)	125(3)	0.272(5)

Table 21. Selected bond lengths [Å] and angles [°] for 8 CCDC 133554 MSS15.

		Distances	
Ru-C(1)	1.979(2)	O(1)-C(9)	1.232(3)
Ru-N(1)	2.046(2)	O(2)-C(9)	1.309(3)
Ru-O(1)	2.1064(16)	O(2)-C(1)	1.505(3)
Ru-N(3)	2.124(2)	C(1)-C(2)	1.330(3)
Ru-N(2)	2.192(2)	C(9)-C(10)	1.527(3)
Ru-P	2.2967(7)		
		Angles	
C(1)-Ru-N(1)	96.92(9)	O(1)-Ru-P	92.74(5)
C(1)-Ru-O(1)	79.63(8)	N(3)-Ru-P	178.04(6)
N(1)-Ru-O(1)	173.37(7)	N(2)-Ru-P	94.02(6)
C(1)-Ru-N(3)	87.17(9)	C(9)-O(1)-Ru	111.85(15)
N(1)-Ru-N(3)	84.94(8)	C(9)-O(2)-C(1)	113.72(19)
O(1)-Ru-N(3)	89.22(8)	C(2)-C(1)-O(2)	112.2(2)
C(1)-Ru-N(2)	171.77(9)	C(2)-C(1)-Ru	137.0(2)
N(1)-Ru-N(2)	86.68(8)	O(2)-C(1)-Ru	110.52(15)
O(1)-Ru-N(2)	96.03(7)	O(1)-C(9)-O(2)	123.5(2)
N(3)-Ru-N(2)	85.78(8)	O(1)-C(9)-C(10)	120.9(2)
C(1)-Ru-P	93.17(7)	O(2)-C(9)-C(10)	115.5(2)
N(1)-Ru-P	93.10(6)		

Table 22. Bond lengths [Å] and angles [°] for 8 CCDC 133554 MSS15.

Ru-C(1)	1.979(2)	C(16)-H(16)	0.9300
Ru-N(1)	2.046(2)	C(17)-C(22)	1.358(4)
Ru-O(1)	2.1064(16)	C(17)-C(18)	1.374(4)
Ru-N(3)	2.124(2)	C(18)-C(19)	1.382(5)
Ru-N(2)	2.192(2)	C(18)-H(18)	0.9300
Ru-P	2.2967(7)	C(19)-C(20)	1.361(5)
P-C(32)	1.834(3)	C(19)-H(19)	0.9300
P-C(44)	1.837(3)	C(20)-C(21)	1.344(4)
P-C(38)	1.842(3)	C(20)-H(20)	0.9300
O(1)-C(9)	1.232(3)	C(21)-C(22)	1.382(4)
O(2)-C(9)	1.309(3)	C(21)-H(21)	0.9300
O(2)-C(1)	1.505(3)	C(22)-H(22)	0.9300
N(1)-C(23)	1.332(3)	C(23)-C(24)	1.394(4)
N(1)-N(4)	1.370(3)	C(23)-H(23)	0.9300
N(2)-C(26)	1.324(3)	C(24)-C(25)	1.345(4)
N(2)-N(5)	1.369(3)	C(24)-H(24)	0.9300
N(3)-C(29)	1.327(3)	C(25)-H(25)	0.9300
N(3)-N(6)	1.359(3)	C(26)-C(27)	1.384(4)
N(4)-C(25)	1.357(3)	C(26)-H(26)	0.9300
N(4)-B	1.546(4)	C(27)-C(28)	1.361(4)
N(5)-C(28)	1.338(3)	C(27)-H(27)	0.9300
N(5)-B	1.530(4)	C(28)-H(28)	0.9300
N(6)-C(31)	1.334(4)	C(29)-C(30)	1.384(4)
N(6)-B	1.539(4)	C(29)-H(29)	0.9300
C(1)-C(2)	1.330(3)	C(30)-C(31)	1.363(4)
C(2)-C(3)	1.467(3)	C(30)-H(30)	0.9300
C(2)-H(2)	0.9300	C(31)-H(31)	0.9300
C(3)-C(8)	1.382(4)	C(32)-C(37)	1.358(4)
C(3)-C(4)	1.391(4)	C(32)-C(33)	1.377(4)
C(4)-C(5)	1.386(4)	C(33)-C(34)	1.393(4)
C(4)-H(4)	0.9300	C(33)-H(33)	0.9300
C(5)-C(6)	1.366(5)	C(34)-C(35)	1.344(4)
C(5)-H(5)	0.9300	C(34)-H(34)	0.9300
C(6)-C(7)	1.361(4)	C(35)-C(36)	1.362(5)
C(6)-H(6)	0.9300	C(35)-H(35)	0.9300
C(7)-C(8)	1.384(4)	C(36)-C(37)	1.377(5)
C(7)-H(7)	0.9300	C(36)-H(36)	0.9300
C(8)-H(8)	0.9300	C(37)-H(37)	0.9300
C(9)-C(10)	1.527(3)	C(38)-C(39)	1.377(4)
C(10)-C(11)	1.509(4)	C(38)-C(43)	1.384(4)
C(10)-C(17)	1.528(4)	C(39)-C(40)	1.400(4)
C(10)-H(10)	0.9800	C(39)-H(39)	0.9300
C(11)-C(16)	1.367(4)	C(40)-C(41)	1.342(5)
C(11)-C(12)	1.374(4)	C(40)-H(40)	0.9300
C(12)-C(13)	1.385(5)	C(41)-C(42)	1.366(4)
C(12)-H(12)	0.9300	C(41)-H(41)	0.9300
C(13)-C(14)	1.355(5)	C(42)-C(43)	1.383(4)
C(13)-H(13)	0.9300	C(42)-H(42)	0.9300
C(14)-C(15)	1.353(5)	C(43)-H(43)	0.9300
C(14)-H(14)	0.9300	C(44)-C(49)	1.378(4)
C(15)-C(16)	1.374(4)	C(44)-C(45)	1.391(4)
C(15)-H(15)	0.9300	C(45)-C(46)	1.384(4)

C(45)-H(45)	0.9300
C(46)-C(47)	1.357(5)
C(46)-H(46)	0.9300
C(47)-C(48)	1.365(5)
C(47)-H(47)	0.9300
C(48)-C(49)	1.396(4)
C(48)-H(48)	0.9300
C(49)-H(49)	0.9300
C(51)-C(52)	1.3900
C(51)-C(56)	1.3900
C(51)-C(50)	1.5381
C(52)-C(53)	1.3900
C(52)-H(52)	0.9300
C(53)-C(54)	1.3900
C(53)-H(53)	0.9300
C(54)-C(55)	1.3900
C(54)-H(54)	0.9300
C(55)-C(56)	1.3900
C(55)-H(55)	0.9300
C(56)-H(56)	0.9300
C(50)-H(50A)	0.9600
C(50)-H(50B)	0.9600
C(50)-H(50C)	0.9600
C(61)-C(62)	1.3900
C(61)-C(66)	1.3900
C(61)-C(60)	1.5384
C(62)-C(63)	1.3900
C(62)-H(62)	0.9300
C(63)-C(64)	1.3900
C(63)-H(63)	0.9300
C(64)-C(65)	1.3900
C(64)-H(64)	0.9300
C(65)-C(66)	1.3900
C(65)-H(65)	0.9300
C(66)-H(66)	0.9300
C(60)-H(60A)	0.9600
C(60)-H(60B)	0.9600
C(60)-H(60C)	0.9600

C(1)-Ru-N(1)	96.92(9)
C(1)-Ru-O(1)	79.63(8)
N(1)-Ru-O(1)	173.37(7)
C(1)-Ru-N(3)	87.17(9)
N(1)-Ru-N(3)	84.94(8)
O(1)-Ru-N(3)	89.22(8)
C(1)-Ru-N(2)	171.77(9)
N(1)-Ru-N(2)	86.68(8)
O(1)-Ru-N(2)	96.03(7)
N(3)-Ru-N(2)	85.78(8)
C(1)-Ru-P	93.17(7)
N(1)-Ru-P	93.10(6)
O(1)-Ru-P	92.74(5)
N(3)-Ru-P	178.04(6)
N(2)-Ru-P	94.02(6)

C(32)-P-C(44)	101.96(12)
C(32)-P-C(38)	101.32(13)
C(44)-P-C(38)	101.76(12)
C(32)-P-Ru	115.44(9)
C(44)-P-Ru	117.16(9)
C(38)-P-Ru	116.72(9)
C(9)-O(1)-Ru	111.85(15)
C(9)-O(2)-C(1)	113.72(19)
C(23)-N(1)-N(4)	106.4(2)
C(23)-N(1)-Ru	135.09(19)
N(4)-N(1)-Ru	118.49(16)
C(26)-N(2)-N(5)	106.1(2)
C(26)-N(2)-Ru	136.6(2)
N(5)-N(2)-Ru	117.30(16)
C(29)-N(3)-N(6)	106.5(2)
C(29)-N(3)-Ru	134.1(2)
N(6)-N(3)-Ru	119.30(17)
C(25)-N(4)-N(1)	108.6(2)
C(25)-N(4)-B	129.0(3)
N(1)-N(4)-B	122.3(2)
C(28)-N(5)-N(2)	109.4(2)
C(28)-N(5)-B	130.2(3)
N(2)-N(5)-B	120.4(2)
C(31)-N(6)-N(3)	108.9(2)
C(31)-N(6)-B	130.6(3)
N(3)-N(6)-B	119.9(2)
N(5)-B-N(6)	108.5(2)
N(5)-B-N(4)	108.0(2)
N(6)-B-N(4)	106.8(2)
C(2)-C(1)-O(2)	112.2(2)
C(2)-C(1)-Ru	137.0(2)
O(2)-C(1)-Ru	110.52(15)
C(1)-C(2)-C(3)	135.3(3)
C(1)-C(2)-H(2)	112.3
C(3)-C(2)-H(2)	112.3
C(8)-C(3)-C(4)	117.2(3)
C(8)-C(3)-C(2)	125.4(3)
C(4)-C(3)-C(2)	117.4(3)
C(5)-C(4)-C(3)	121.6(3)
C(5)-C(4)-H(4)	119.2
C(3)-C(4)-H(4)	119.2
C(6)-C(5)-C(4)	120.0(3)
C(6)-C(5)-H(5)	120.0
C(4)-C(5)-H(5)	120.0
C(7)-C(6)-C(5)	119.1(3)
C(7)-C(6)-H(6)	120.5
C(5)-C(6)-H(6)	120.5
C(6)-C(7)-C(8)	121.6(3)
C(6)-C(7)-H(7)	119.2
C(8)-C(7)-H(7)	119.2
C(3)-C(8)-C(7)	120.5(3)
C(3)-C(8)-H(8)	119.8
C(7)-C(8)-H(8)	119.8
O(1)-C(9)-O(2)	123.5(2)

O(1)-C(9)-C(10)	120.9(2)
O(2)-C(9)-C(10)	115.5(2)
C(11)-C(10)-C(9)	114.6(2)
C(11)-C(10)-C(17)	112.3(2)
C(9)-C(10)-C(17)	112.7(2)
C(11)-C(10)-H(10)	105.4
C(9)-C(10)-H(10)	105.4
C(17)-C(10)-H(10)	105.4
C(16)-C(11)-C(12)	118.2(3)
C(16)-C(11)-C(10)	121.9(3)
C(12)-C(11)-C(10)	119.8(3)
C(11)-C(12)-C(13)	120.4(4)
C(11)-C(12)-H(12)	119.8
C(13)-C(12)-H(12)	119.8
C(14)-C(13)-C(12)	119.4(4)
C(14)-C(13)-H(13)	120.3
C(12)-C(13)-H(13)	120.3
C(15)-C(14)-C(13)	121.3(4)
C(15)-C(14)-H(14)	119.4
C(13)-C(14)-H(14)	119.4
C(14)-C(15)-C(16)	118.9(4)
C(14)-C(15)-H(15)	120.6
C(16)-C(15)-H(15)	120.5
C(11)-C(16)-C(15)	121.7(3)
C(11)-C(16)-H(16)	119.1
C(15)-C(16)-H(16)	119.2
C(22)-C(17)-C(18)	117.8(3)
C(22)-C(17)-C(10)	123.8(3)
C(18)-C(17)-C(10)	118.3(3)
C(17)-C(18)-C(19)	120.7(3)
C(17)-C(18)-H(18)	119.6
C(19)-C(18)-H(18)	119.7
C(20)-C(19)-C(18)	120.0(4)
C(20)-C(19)-H(19)	120.0
C(18)-C(19)-H(19)	120.0
C(21)-C(20)-C(19)	119.9(4)
C(21)-C(20)-H(20)	120.0
C(19)-C(20)-H(20)	120.0
C(20)-C(21)-C(22)	119.9(4)
C(20)-C(21)-H(21)	120.1
C(22)-C(21)-H(21)	120.0
C(17)-C(22)-C(21)	121.6(3)
C(17)-C(22)-H(22)	119.2
C(21)-C(22)-H(22)	119.2
N(1)-C(23)-C(24)	110.3(3)
N(1)-C(23)-H(23)	124.8
C(24)-C(23)-H(23)	124.8
C(25)-C(24)-C(23)	105.4(3)
C(25)-C(24)-H(24)	127.3
C(23)-C(24)-H(24)	127.3
N(4)-C(25)-C(24)	109.2(3)
N(4)-C(25)-H(25)	125.4
C(24)-C(25)-H(25)	125.4
N(2)-C(26)-C(27)	110.7(3)
N(2)-C(26)-H(26)	124.6
C(27)-C(26)-H(26)	124.6
C(28)-C(27)-C(26)	105.1(3)
C(28)-C(27)-H(27)	127.5
C(26)-C(27)-H(27)	127.5
N(5)-C(28)-C(27)	108.7(3)
N(5)-C(28)-H(28)	125.6
C(27)-C(28)-H(28)	125.6
N(3)-C(29)-C(30)	110.7(3)
N(3)-C(29)-H(29)	124.6
C(30)-C(29)-H(29)	124.6
C(31)-C(30)-C(29)	104.3(3)
C(31)-C(30)-H(30)	127.9
C(29)-C(30)-H(30)	127.9
N(6)-C(31)-C(30)	109.6(3)
N(6)-C(31)-H(31)	125.2
C(30)-C(31)-H(31)	125.2
C(37)-C(32)-C(33)	116.7(3)
C(37)-C(32)-P	123.6(2)
C(33)-C(32)-P	119.6(2)
C(32)-C(33)-C(34)	121.8(3)
C(32)-C(33)-H(33)	119.1
C(34)-C(33)-H(33)	119.1
C(35)-C(34)-C(33)	120.0(3)
C(35)-C(34)-H(34)	120.0
C(33)-C(34)-H(34)	120.0
C(34)-C(35)-C(36)	118.7(4)
C(34)-C(35)-H(35)	120.6
C(36)-C(35)-H(35)	120.6
C(35)-C(36)-C(37)	121.2(4)
C(35)-C(36)-H(36)	119.4
C(37)-C(36)-H(36)	119.4
C(32)-C(37)-C(36)	121.5(3)
C(32)-C(37)-H(37)	119.3
C(36)-C(37)-H(37)	119.3
C(39)-C(38)-C(43)	117.8(3)
C(39)-C(38)-P	123.6(2)
C(43)-C(38)-P	118.5(2)
C(38)-C(39)-C(40)	120.2(3)
C(38)-C(39)-H(39)	119.9
C(40)-C(39)-H(39)	119.9
C(41)-C(40)-C(39)	121.2(4)
C(41)-C(40)-H(40)	119.4
C(39)-C(40)-H(40)	119.4
C(40)-C(41)-C(42)	119.4(3)
C(40)-C(41)-H(41)	120.3
C(42)-C(41)-H(41)	120.3
C(41)-C(42)-C(43)	120.5(3)
C(41)-C(42)-H(42)	119.7
C(43)-C(42)-H(42)	119.7
C(42)-C(43)-C(38)	120.9(3)
C(42)-C(43)-H(43)	119.5
C(38)-C(43)-H(43)	119.5
C(49)-C(44)-C(45)	117.9(3)

C(49)-C(44)-P	119.4(2)	C(55)-C(56)-H(56)	120.0
C(45)-C(44)-P	122.7(2)	C(51)-C(56)-H(56)	120.0
C(46)-C(45)-C(44)	121.0(3)	C(51)-C(50)-H(50A)	109.5
C(46)-C(45)-H(45)	119.5	C(51)-C(50)-H(50B)	109.5
C(44)-C(45)-H(45)	119.5	H(50A)-C(50)-H(50B)	109.5
C(47)-C(46)-C(45)	120.2(3)	C(51)-C(50)-H(50C)	109.5
C(47)-C(46)-H(46)	119.9	H(50A)-C(50)-H(50C)	109.5
C(45)-C(46)-H(46)	119.9	H(50B)-C(50)-H(50C)	109.5
C(46)-C(47)-C(48)	120.1(3)	C(62)-C(61)-C(66)	120.0
C(46)-C(47)-H(47)	119.9	C(62)-C(61)-C(60)	119.9
C(48)-C(47)-H(47)	119.9	C(66)-C(61)-C(60)	118.8
C(47)-C(48)-C(49)	120.2(3)	C(61)-C(62)-C(63)	120.0
C(47)-C(48)-H(48)	119.9	C(61)-C(62)-H(62)	120.0
C(49)-C(48)-H(48)	119.9	C(63)-C(62)-H(62)	120.0
C(44)-C(49)-C(48)	120.6(3)	C(64)-C(63)-C(62)	120.0
C(44)-C(49)-H(49)	119.7	C(64)-C(63)-H(63)	120.0
C(48)-C(49)-H(49)	119.7	C(62)-C(63)-H(63)	120.0
C(52)-C(51)-C(56)	120.0	C(65)-C(64)-C(63)	120.0
C(52)-C(51)-C(50)	117.1	C(65)-C(64)-H(64)	120.0
C(56)-C(51)-C(50)	122.9	C(63)-C(64)-H(64)	120.0
C(51)-C(52)-C(53)	120.0	C(64)-C(65)-C(66)	120.0
C(51)-C(52)-H(52)	120.0	C(64)-C(65)-H(65)	120.0
C(53)-C(52)-H(52)	120.0	C(66)-C(65)-H(65)	120.0
C(54)-C(53)-C(52)	120.0	C(65)-C(66)-C(61)	120.0
C(54)-C(53)-H(53)	120.0	C(65)-C(66)-H(66)	120.0
C(52)-C(53)-H(53)	120.0	C(61)-C(66)-H(66)	120.0
C(53)-C(54)-C(55)	120.0	C(61)-C(60)-H(60A)	109.5
C(53)-C(54)-H(54)	120.0	C(61)-C(60)-H(60B)	109.5
C(55)-C(54)-H(54)	120.0	H(60A)-C(60)-H(60B)	109.5
C(56)-C(55)-C(54)	120.0	C(61)-C(60)-H(60C)	109.5
C(56)-C(55)-H(55)	120.0	H(60A)-C(60)-H(60C)	109.5
C(54)-C(55)-H(55)	120.0	H(60B)-C(60)-H(60C)	109.5
C(55)-C(56)-C(51)	120.0		

Table 23. Anisotropic displacement parameters ($Å^2 x 10^4$) for 8_CCDC 133554_MSS15. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru	444(1)	330(1)	430(1)	4(1)	101(1)	38(1)
P	454(4)	371(4)	462(4)	-14(3)	114(3)	47(3)
O(1)	543(12)	359(10)	456(10)	-13(8)	99(9)	62(9)
O(2)	603(12)	366(10)	481(10)	15(8)	138(9)	89(9)
N(1)	446(13)	363(13)	502(13)	23(10)	142(11)	47(11)
N(2)	539(15)	455(14)	490(13)	24(11)	93(12)	55(12)
N(3)	476(13)	431(13)	543(13)	-9(12)	104(11)	30(13)
N(4)	531(15)	398(13)	594(14)	90(11)	196(12)	104(12)
N(5)	576(15)	461(14)	524(14)	53(11)	39(12)	98(12)
N(6)	431(14)	552(17)	701(16)	27(13)	63(12)	70(13)
B	600(20)	510(20)	610(20)	37(17)	120(19)	37(18)
C(1)	427(15)	335(14)	504(15)	-12(12)	108(13)	32(12)
C(2)	549(18)	422(16)	525(16)	-5(13)	158(14)	13(13)
C(3)	493(17)	512(18)	437(15)	23(13)	80(13)	-110(15)
C(4)	760(20)	640(20)	589(19)	12(16)	225(17)	-106(18)
C(5)	930(30)	980(30)	560(20)	40(20)	300(20)	-260(20)
C(6)	800(30)	990(30)	580(20)	250(20)	30(20)	-270(20)
C(7)	740(20)	730(20)	730(20)	253(19)	-10(20)	-31(19)
C(8)	587(19)	660(20)	526(17)	103(16)	94(15)	19(17)
C(9)	425(16)	372(15)	541(17)	-59(13)	111(14)	1(13)
C(10)	506(17)	400(16)	619(18)	-11(14)	180(15)	47(14)
C(11)	570(19)	390(16)	574(18)	-80(14)	39(16)	125(15)
C(12)	720(20)	630(20)	930(30)	-70(20)	-90(20)	81(19)
C(13)	880(30)	1010(30)	920(30)	-230(30)	-270(30)	260(30)
C(14)	1440(50)	900(30)	550(20)	-100(20)	-120(30)	590(30)
C(15)	1150(30)	730(30)	700(20)	140(20)	240(20)	290(20)
C(16)	750(20)	600(20)	670(20)	66(17)	113(18)	192(19)
C(17)	620(20)	348(15)	466(16)	-27(12)	96(15)	31(14)
C(18)	830(30)	750(20)	990(30)	-270(20)	230(20)	80(20)
C(19)	1150(40)	940(30)	1050(30)	-540(30)	240(30)	-10(30)
C(20)	1120(30)	710(30)	790(30)	-240(20)	-20(30)	-100(30)
C(21)	770(20)	630(20)	780(20)	45(19)	-50(20)	-40(20)
C(22)	660(20)	516(19)	620(19)	-55(15)	71(17)	40(17)
C(23)	600(19)	438(17)	528(16)	-19(14)	194(15)	15(15)
C(24)	850(20)	431(18)	660(20)	-51(15)	338(19)	83(17)
C(25)	720(20)	414(18)	760(20)	84(16)	340(19)	184(16)
C(26)	750(20)	670(20)	481(17)	22(15)	200(17)	88(18)
C(27)	1070(30)	770(20)	503(18)	160(17)	190(20)	180(20)
C(28)	850(20)	570(20)	513(18)	113(15)	23(18)	163(18)
C(29)	620(20)	454(18)	780(20)	18(16)	232(18)	-42(16)
C(30)	560(20)	700(20)	1080(30)	-70(20)	180(20)	-149(19)
C(31)	416(19)	780(30)	1010(30)	-20(20)	54(18)	9(18)
C(32)	457(17)	478(17)	541(16)	26(14)	163(14)	-6(15)
C(33)	650(20)	549(19)	770(20)	145(16)	287(18)	29(17)
C(34)	780(20)	640(20)	1080(30)	310(20)	330(20)	120(20)
C(35)	1130(30)	840(30)	1680(40)	630(30)	750(30)	180(30)
C(36)	1210(40)	1140(40)	2460(60)	780(40)	1270(40)	270(30)
C(37)	800(30)	740(30)	1600(40)	430(30)	660(30)	200(20)